Bose Einstein condensate in the Lowest Landau Level: Hamiltonian dynamics

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Abstract

In a previous article with A. Aftalion and X. Blanc, it was shown that the hypercontractivity property of the dilation semigroup in spaces of entire functions was a key ingredient in the study of the Lowest Landau Level model for fast rotating Bose Einstein condensates. That former work was concerned with the stationnary constrained variational problem. This article is about the nonlinear Hamiltonian dynamics and the spectral stability of the constrained minima with motivations arising from the description of Tkatchenko modes of Bose-Einstein condensates. Again the hypercontractivity property provides a very strong control of the nonlinear term in the dynamical analysis.

1 Introduction

The Lowest Landau Level energy functional of rapidly rotating Bose-Einstein condensates in a harmonic trap can be written as

$$G^h(f) = \int_{\mathbb{C}} |z|^2 \left| f(z) e^{-\frac{|z|^2}{2h}} \right|^2 + \frac{Na\Omega_h^2}{2} \left| f(z)\ e^{-\frac{|z|^2}{2h}} \right|^4 L(dz)\,. \tag{1.1}$$

The number N of atoms in the condensate and the scattering length a are fixed and $h = \sqrt{1-\Omega_h^2}$, where Ω_h is the ratio of two rotational velocities, is a small parameter. Here and in the sequel $L(dz)$ denotes the Lebesgue measure on $\mathbb{C} \sim \mathbb{R}^2$. In this scaling, the set of admissible f in the Lowest Landau Level approximation, is the semiclassical

Fock-Bargmann space

$$\mathcal{F}_h = \left\{ f \in L^2(\mathbb{C}, e^{-\frac{|z|^2}{h}} L(dz)),\ \text{s.t } f \text{ entire} \right\} \tag{1.2}$$

$$\text{with} \qquad \|f\|^2_{\mathcal{F}_h} = \int_{\mathbb{C}} |f(z)|^2 e^{-\frac{|z|^2}{h}} L(dz)\ . \tag{1.3}$$

The equilibrium states which are experimentally observed are within this modelling the solution of the constrained minimization problem

$$\inf \left\{ G^h(f),\ f \in \mathcal{F}_h,\ \|f\|_{\mathcal{F}_h} = 1 \right\}\ . \tag{1.4}$$

We follow the presentation of [ABN1, ABN2] and additional information about the physics of the problem can be found in [ARVK, Aft, ABD, Ho, WBP].
This article focuses on the nonlinear Hamiltonian dynamics

$$i\partial_t f = 2\nabla_{\overline{f}} G^h(f) \tag{1.5}$$

and on the spectral analysis of the linearized Hamiltonian around an equilibrium configuration. This last problem is motivated by the experimental and numerical study of the vibration modes of condensates, also known as Tkachenko modes, which can be found in the physics literature [BWCB, SCEMC, Son].

More precisely, after specifying the functional framework and the results of [ABN2] about the minimization problem, the following topics will be studied:

1. Owing the hypercontractivity property already used in [ABN2], the Hamiltonian flow associated with the nonlinear equation (1.5) will be globally defined on $\mathcal{F}_h$.

2. The spectral stability,[1] of constrained minimizers will be proved after a natural modification of the energy functional. Since a minimum of the functional G^h on the sphere, $\left\{\|f\|_{\mathcal{F}_h} = 1\right\}$, is not always a local minimum of G^h and due to some degeneracy related with the rotational invariance, the spectral stability is better studied by considering a modified energy

$$G^h_{\Phi_0,\Phi_1}(f) = G^h(f) + \Phi_0(\|f\|^2_{\mathcal{F}_h}) + \Phi_1(\langle f \mid zh\partial_z f\rangle_{\mathcal{F}_h})$$

in which the two additional terms are functions of quantities left invariant by the Hamiltonian dynamics. This change of energy functional, amounts to a simple explicit time-dependent gauge transformation $f_{\Phi_0,\Phi_1}(z,t) = e^{i\alpha_1 t} f(e^{i\alpha_2 t} z, t)$ where the real numbers α_1, α_2 are determined by the choice of Φ_0, Φ_1, and the initial data $f(z, t = 0) \in \mathcal{F}_h$. A good choice of the function Φ_0, Φ_1 allows to prove that the spectrum of the modified linearized Hamiltonian is purely imaginary. From the physical point of view, the introduction of an artificially modified dynamics is related with the idea that one is interested in the linearized dynamics up to uniform solid rotations of the whole condensate. A good intuitive picture is provided by the vibration modes of a swinging bell.

[1] i.e. the spectrum of the linearized Hamiltonian is purely imaginary

3. The relevance of numerical approximations is considered: the numerical simulations in [ABD] consist in minimizing the energy G^h on a space of polynomials with bounded degree, instead of the space $\mathcal{F}_h$. It was checked in [ABN2] that when the degree of the polynomials is taken sufficiently large, the solution to the finite dimensional problem provides a suitable approximation of the minimizer in $\mathcal{F}_h$. Here it is proved that a similar result holds for the linearized Hamiltonian in a norm resolvent sense. We end with some comments about the numerical stability of the spectral elements in such an approximation, by pointing out that the linearized Hamiltonian is a non anti-adjoint operator with a purely imaginary spectrum.

The appendix gathers standard tools about the classical Hamiltonian dynamics in infinite dimension and some results are adapted to our specific framework.

2 Preliminaries

In this section, we set up the functional framework. The basic tools introduced in [ABN2] and the initial result on the minimization problem (1.4) are reviewed. Then, the Kaehler structure of $\mathcal{F}_h$, which is the combination of its (real) euclidean structure and its (real) symplectic structure and which is the natural framework for the study of the Hessian and the linearized Hamiltonian flow, is explicitely written. Finally, the Hessian of the functional G^h is computed and an estimate is given for $\mathrm{H}ess\, G^h(f)$ when f is a solution to (1.4).

2.1 The minimization problem

Here is a very short review of [ABN2]. The Bargmann transform (see for example [Bar, Fol, Mar]) is used with the following normalization

$$[B_h\varphi](z) = \frac{1}{(\pi h)^{3/4}} e^{\frac{z^2}{2h}} \int_{\mathbb{R}} e^{-\frac{(\sqrt{2}z-y)^2}{2h}} \varphi(y)\; dy\,,$$

with $z = \frac{x-i\xi}{\sqrt{2}} \in \mathbb{C}$ and $\varphi \in \mathcal{S}'(\mathbb{R})$. It defines a unitary operator $B_h : L^2(\mathbb{R}, dy) \to \mathcal{F}_h$ and the orthogonal projection $\Pi_h = B_h B_h^* : L^2(\mathbb{C}, e^{-\frac{|z|^2}{h}} L(dz)) \to \mathcal{F}_h$ is given by

$$[\Pi_h f](z) = [B_h B_h^* f](z) = \frac{1}{\pi h} \int_{\mathbb{C}} e^{\frac{z\overline{z'}}{h}} e^{-\frac{|z'|^2}{h}} f(z')\; L(dz')\,.$$

The harmonic oscillator quantum Hamiltonian (or number operator in the Fock representation) given by:

$$\begin{aligned} \tilde{N}_h &= \frac{1}{2}(-h^2\partial_y^2 + y^2 - h) \\ D(\tilde{N}_h) &= \left\{u \in L^2(\mathbb{R}, dy),\; y^\alpha \partial_y^\beta u \in L^2(\mathbb{R}, dy),\; \alpha+\beta \le 2\right\}, \end{aligned}$$

is transformed into the generator of dilations:

$$N_h = B_h \tilde{N}_h B_h^* = z(h\partial_z)\,.$$

An element $f = B_h\varphi$ of $\mathcal{F}_h$ considered as an element of $L^2(\mathbb{C}, e^{-\frac{|z|^2}{h}}L(dz))$, satisfies

$$h\partial_z f = h\partial_z(\Pi_h f) = \Pi_h(\overline{z}f)\ .$$

For the spectral resolution of these two operators, the basis of normalized Hermite functions $(c_n H_n(y))_{n\in\mathbb{N}}$ is tranformed via B_h into the the basis of monomials $(c_n z^n)_{n\in\mathbb{N}}$. Then the spaces

$$\mathcal{F}_h^s = \left\{ f \text{ entire, s.t. } \int_{\mathbb{C}} \langle z\rangle^{2s}|f(z)|^2 e^{-\frac{|z|^2}{h}} L(dz) < \infty \right\}, \tag{2.1}$$

where $\langle z\rangle = \sqrt{1+|z|^2}$ can identified constructed via the spectral resolution of N_h. The union $\cup_{z\in\mathbb{R}}\mathcal{F}_h^s$ is nothing but $B_h\left[\mathcal{S}'(\mathbb{R})\right]$ and $\mathcal{F}_h^s$ is compactly embedded in $\mathcal{F}_h$ as soon as $s>0$.
Another property which will be used also in this article, is the next consequence of the hypercontractivity property of the semigroup $(e^{-tN_1})_{t>0}$ (see for example [Car, Gro, Nel]):

Lemma 2.1. *[ABN2] The quantity*

$$\int_{\mathbb{C}} \overline{f_1(z)f_2(z)} f_3(z)f_4(z)e^{\frac{-2|z|^2}{h}}\ L(dz)$$

defines a continuous $(2,2)$*-linear functional* [2] *on* $\mathcal{F}_h$ *with norm smaller than* $\frac{1}{2\pi h}$. *Hence for any* $\alpha,\beta\in\{0,1,2\}$, *the* $\partial_{\overline{f}}^{\alpha}\partial_f^{\beta}$ *derivative of the functional*

$$f \to \int_{\mathbb{C}} |f(z)|^4\, e^{\frac{-2|z|^2}{h}}\ L(dz)$$

defines a continuous $(2-\alpha,2-\beta)$*-linear mapping from* $\mathcal{F}_h$ *into* $\overline{\mathcal{F}_h}^{\hat{\otimes}\alpha}\hat{\otimes}\mathcal{F}_h^{\hat{\otimes}\beta}$ *with norm* $\frac{4}{2\pi h(2-\alpha)!(2-\beta)!}$.

The above Lemma and the compactness of the imbedding $\mathcal{F}_h^1\subset\mathcal{F}_h$ lead naturally to the next result (see the proof in [ABN2])

Theorem 2.2. *[ABN2] For any fixed* $h>0$, *the minimization problem* (1.4) *admits a solution in* $\mathcal{F}_h^1$. *Any minimizer is a solution to the Euler-Lagrange equation*

$$\Pi_h\left[\left(|z|^2 + Na\Omega_h^2 e^{-\frac{|z|^2}{h}}\,|f|^2 - \lambda\right) f\right] = 0 \tag{2.2}$$

[2] A $(2,2)$-linear functional is an $\mathbb{R}$-quadrilinear functional which is $\overline{\mathbb{C}}$-linear with respect to the two first arguments and $\mathbb{C}$-linear with respect to the two last arguments.

where $\lambda \in \mathbb{R}$ is the Lagrange multiplier satisfying the uniform estimates

$$\frac{2\Omega_h}{3}\sqrt{\frac{2Na}{\pi}} < e^h_{LLL} \leq \lambda \leq 2e^h_{LLL} \leq 2\frac{2\Omega_h}{3}\sqrt{\frac{2bNa}{\pi}} + o_{Na}(h^0)\,, \tag{2.3}$$

with

$$e^h_{LLL} = \min\left\{G^h(f)\,, \quad f \in \mathcal{F}_h, \quad \|f\|_{\mathcal{F}_h} = 1\right\}.$$

The Euler-Lagrange equation (2.2) can also be written as

$$zh\partial_z f + Na\Omega_h^2 \Pi_h\left(e^{-\frac{|z|^2}{h}}\,|f|^2\right)\Pi_h f - (\lambda - h)f = 0\,, \tag{2.4}$$

$$\text{or} \qquad zh\partial_z f + \frac{Na\Omega_h^2}{2}\bar{f}(h\partial_z)[f^2(2^{-1}.)] - (\lambda - h)f = 0\,, \tag{2.5}$$

the operator $\bar{f}(h\partial_z)$ being defined as the limit $\lim_{K\to\infty}\sum_{k=0}^K \overline{a_k}(h\partial_z)^k$ if $f(z) = \sum_{k=0}^\infty a_k z^k$.

2.2 The Kaehler structure

The Hessian of the energy functional and the linearized Hamiltonian vector field, are objects associated with the real euclidean structure or with the real symplectic structure of $\mathcal{F}_h$. Some of their properties are more obvious in this presentation. We specify here the Kaehler structure associated with the complex Hilbert space $\mathcal{F}_h$.
The space $\mathcal{F}_h$ can be viewed as a real Hilbert space with the scalar product:

$$\mathbb{R}\mathrm{e}\,\langle f_1\,|\,f_2\rangle_{\mathcal{F}_h}$$

and as a symplectic space with the form

$$\sigma(f_1, f_2) = -\mathcal{I}\mathrm{m}\,\langle f_1\,|\,f_2\rangle_{\mathcal{F}_h}\ .$$

The Euclidean structure on $\mathcal{F}_h$ is more convenient when one studies the second variation, while the symplectic structure will be used in Section 3 for the Hamiltonian flow. These structures are completely clarified once the complex conjugation is defined on $\mathcal{F}_h$. The simplest way of writing can be done in the orthonormal basis $B_h[H^h_n] = c_{n,h}z^n$ with $c_{n,h} = \frac{1}{(\pi h)^{1/2}h^{n/2}\sqrt{n!}}$. Let

$$f_k = \sum_{n\in\mathbb{N}} f_{k,n}c_{n,h}z^n = \sum_{n\in\mathbb{N}}(f^R_{k,n} + if^I_{k,n})c_{n,h}z^n, \qquad k \in \{1, 2\}$$

we get

$$\langle f_1\,|\,f_2\rangle_{\mathcal{F}_h} = \sum_{n\in\mathbb{N}} \overline{f_{1,n}}f_{2,n}$$

$$\langle f_1\,|\,f_2\rangle_{\mathcal{F}_h,\mathbb{R}} = \sum_{n\in\mathbb{N}} f^R_{1,n}f^R_{2,n} + f^I_{n,1}f^I_{n,2} = \left(f^R_1, f^I_1\right)\begin{pmatrix} f^R_2 \\ f^I_2 \end{pmatrix}\,,$$

$$\text{and} \qquad \sigma(f_1, f_2) = \sum_{n\in\mathbb{N}} f^I_{1,n}f^R_{2,n} - f^R_{1,n}f^I_{2,n} = \left(f^R_1, f^I_1\right)\begin{pmatrix} 0 & \mathrm{Id} \\ -\mathrm{Id} & 0 \end{pmatrix}\begin{pmatrix} f^R_2 \\ f^I_2 \end{pmatrix}.$$

For the real scalar product $\mathbb{R}\mathrm{e}\langle f_1 \,|\, f_2\rangle$, we will use the notation $f_1^T f_2$ which refers to the matrix representation.
The natural definition of $\overline{f}$ (which has to stay in a space of holomorphic functions) follows from the writing $f(z) = \sum_{n\in\mathbb{N}}(f_n^R + if_n^I)c_{n,h}z^n = f_R(z) + if_I(z)$:

$$\overline{f}(z) = \overline{f(\overline{z})}\,.$$

This definition allows to check the relationships (with $f, f_i \in \mathcal{F}_h$ and $v(z,\overline{z})$ non necessarily holomorphic)

$$\langle f_1 \,|\, f_2\rangle_{\mathcal{F}_h} = \int_{\mathbb{C}} e^{-\frac{|z|^2}{h}}\overline{f_1}(\overline{z})f_2(z)\ L(dz)\,, \tag{2.6}$$

$$\overline{\Pi_h[v(z,\overline{z})]} = \Pi_h\left[\overline{v(\overline{z},z)}\right]\,, \qquad \overline{\Pi_h[f(z)]} = \Pi_h\overline{f}\,, \tag{2.7}$$

$$G^h(f) = \int_{\mathbb{C}}\left(e^{-\frac{|z|^2}{h}}\,|z|^2\,\overline{f}(\overline{z})f(z) + \frac{Na\Omega_h^2}{2}e^{-\frac{2|z|^2}{h}}\overline{f}^2(\overline{z})f^2(z)\right)L(dz)\,. \tag{2.8}$$

2.3 Hessian

Of course there are several ways to study the second variation of a function $G^h(f)$, by computing the $(f,\overline{f})$ coordinates or with the coordinates (f_R, f_I) introduced before. The second choice put the stress on the real euclidean structure of $\mathcal{F}_h$ in which the notion of Hessian makes sense.

Proposition 2.3. *Let $f = f_R + if_I \in \mathcal{F}_h$, the Hessian of G^h is a bounded perturbation of $2N_h$ with form domain $\mathcal{F}_h^1 = Q(N_h)$. It defines a closed operator with domain $\mathcal{F}_h^2$ and, after writing $\varphi = \begin{pmatrix}\varphi_R\\ \varphi_I\end{pmatrix}$, is equal to*

$$\mathrm{H}ess\,G^h(f)\varphi = \begin{pmatrix} A & 0\\ 0 & A\end{pmatrix}\varphi + \begin{pmatrix} B & 0\\ 0 & -B\end{pmatrix}\varphi + \begin{pmatrix} 0 & C\\ C & 0\end{pmatrix}\varphi \tag{2.9}$$

where A, B and C are the real operators

$$A\varphi = 2(N_h + h)\varphi + 4Na\Omega_h^2\Pi_h\left(e^{-\frac{|z|^2}{h}}\,|f(z)|^2\right)\Pi_h\varphi \tag{2.10}$$

$$B\varphi = Na\Omega_h^2\Pi_h\left(e^{-\frac{|z|^2}{h}}\,\left[\overline{f}(z)^2 + f(z)^2\right]\varphi(\overline{z})\right) \tag{2.11}$$

$$C\varphi = Na\Omega_h^2\Pi_h\left(e^{-\frac{|z|^2}{h}}i\left[\overline{f}^2(z) - f^2(z)\right]\varphi(\overline{z})\right)\,. \tag{2.12}$$

In the complexified Hilbert space $\mathcal{F}_h \oplus \mathcal{F}_h$, it defines a real self-adjoint operator which has a compact resolvent (and therefore a discrete spectrum going to infinity) and whose spectrum is bounded from below by $-C_0h^{-1}\|f\|^2$.

Remark 2.4. ***a)*** *An operator $\mathcal{A}$ is said to be real when $\overline{\varphi}=\varphi$ implies $\overline{\mathcal{A}\varphi}=\mathcal{A}\varphi$. This definition is used in $\mathcal{F}_h$ with the previous definition of the conjugation $f\to\overline{f}$ and in the complexified space $\mathcal{F}_h\oplus\mathcal{F}_h$, where the conjugation is defined componentwise.*
b) *Beside the conservation of reality, the explicit expression will also be useful in the final discussion of Subsection 4.3.*

Proof: The last expression of $G^h(f_R+if_I)$ suggests to start with the second variation with respect to f and $\overline{f}$:

$$\begin{aligned}
G_2 &= (\varphi_R,\varphi_I)\mathrm{Hess}\,G^h(f)\begin{pmatrix}\varphi_R\\ \varphi_I\end{pmatrix}\\
&= 2\partial_{\overline{f}}\partial_f G^h(f).\overline{\varphi}.\varphi+\partial_f\partial_f G^h(f).\varphi.\varphi+\partial_{\overline{f}}\partial_{\overline{f}}G^h(f).\overline{\varphi}.\overline{\varphi}\\
&= 2\left\langle\varphi\,|\,(N_h+h)\varphi\right\rangle_{\mathcal{F}_h}+4Na\Omega_h^2\int_{\mathbb{C}}e^{-\frac{2|z|^2}{h}}\overline{\varphi}(\overline{z})\,|f|^2\,\varphi(z)\;L(dz)\\
&\quad +Na\Omega_h^2\int_{\mathbb{C}}e^{-\frac{2|z|^2}{h}}\overline{f}^2(\overline{z})\varphi^2(z)\;L(dz)+Na\Omega_h^2\int_{\mathbb{C}}e^{-\frac{2|z|^2}{h}}\overline{\varphi}^2(\overline{z})f^2(z)\;L(dz),
\end{aligned}$$

hence

$$\begin{aligned}
G_2 &= \left\langle\varphi_R\,\middle|\,\left[2(N_h+h)+4Na\Omega_h\Pi_h\left(e^{-\frac{|z|^2}{h}}\,|f|^2\right)\Pi_h\right]\varphi_R\right\rangle_{\mathcal{F}_h}\\
&\quad+\left\langle\varphi_I\,\middle|\,\left[2(N_h+h)+4Na\Omega_h\Pi_h\left(e^{-\frac{|z|^2}{h}}\,|f|^2\right)\Pi_h\right]\varphi_I\right\rangle_{\mathcal{F}_h}\\
&\quad+Na\Omega_h^2\int_{\mathbb{C}}e^{-\frac{2|z|^2}{h}}\overline{f}^2(\overline{z})\left[\varphi_R(z)^2-\varphi_I(z)^2+2i\varphi_R(z)\varphi_I(z)\right]\;L(dz)\\
&\quad+Na\Omega_h^2\int_{\mathbb{C}}e^{-\frac{2|z|^2}{h}}f^2(z)\left[\varphi_R(\overline{z})^2-\varphi_I(\overline{z})^2-2i\varphi_R(\overline{z})\varphi_I(\overline{z})\right]\;L(dz).
\end{aligned}$$

We thus get:

$$\begin{aligned}
G_2 &= \left\langle\varphi_R\,|\,A\varphi_R\right\rangle_{\mathcal{F}_h}+\left\langle\varphi_I\,|\,A\varphi_I\right\rangle_{\mathcal{F}_h}\\
&\quad+Na\Omega_h^2\int_{\mathbb{C}}e^{-\frac{2|z|^2}{h}}\left[\overline{f}(z)^2+f(z)^2\right]\varphi_R^2(\overline{z})\;L(dz)\\
&\quad-Na\Omega_h^2\int_{\mathbb{C}}e^{-\frac{2|z|^2}{h}}\left[\overline{f}(z)^2+f(z)^2\right]\varphi_I^2(\overline{z})\;L(dz)\\
&\quad+Na\Omega_h^2\int_{\mathbb{C}}e^{-\frac{2|z|^2}{h}}i\left[\overline{f}(z)^2-f(z)^2\right]\varphi_I(\overline{z})\varphi_R(\overline{z})\;L(dz)\\
&\quad+Na\Omega_h^2\int_{\mathbb{C}}e^{-\frac{2|z|^2}{h}}i\left[\overline{f}(z)^2-f(z)^2\right]\varphi_R(\overline{z})\varphi_I(\overline{z})\;L(dz)\,.
\end{aligned}$$

The functions φ_R and φ_I are real elements of $\mathcal{F}_h$ and the relations

$$\overline{\varphi_{R,I}(z)}=\varphi_{R,I}(\overline{z})$$

lead to

$$\begin{aligned}(\varphi_R,\varphi_I)\mathrm{H}ess\, G^h(f)\begin{pmatrix}\varphi_R\\ \varphi_I\end{pmatrix} &= \langle \varphi_R\,|\,A\varphi_R\rangle_{\mathcal{F}_h}+\langle \varphi_I\,|\,A\varphi_I\rangle_{\mathcal{F}_h}\\ &\quad+\langle \varphi_R\,|\,B\varphi_R\rangle_{\mathcal{F}_h}-\langle \varphi_I\,|\,B\varphi_I\rangle_{\mathcal{F}_h}\\ &\quad+\langle \varphi_R\,|\,C\varphi_I\rangle_{\mathcal{F}_h}+\langle \varphi_I\,|\,C\varphi_R\rangle_{\mathcal{F}_h}\,.\end{aligned}$$

The expression of $\mathrm{H}ess\, G^h$ is deduced from this once A, B and C are real operators. This is a straightforward consequence of (2.7). Lemma 2.1 implies that $\mathrm{H}ess\, G^h(f)-2N_h$ is a bounded self-adjoint operator with a norm controlled by $C_0h^{-1}\left\|f\right\|^2_{\mathcal{F}_h}$. $\square$

Proposition 2.5. *Assume that $f\in\mathcal{F}^1_h$ is a solution to the minimization problem (1.4) and of the Euler-Lagrange equation (2.2) with Lagrange multiplier $\lambda>0$. Then we have*

$$P_{f^\perp}\mathrm{H}ess\, G^h(f)P_{f^\perp}\geq 2\lambda P_{f^\perp},$$

where $P_{f^\perp}$ denotes the orthogonal projector on $f^\perp$ for the (real) euclidean structure on $\mathcal{F}_h$.

Proof: The result is standard for finite dimensional problems. We write a proof in order to check that Lemma 2.1 provides the suitable norm estimates. Since the derivatives of G^h with order larger than 2 are bounded according to Lemma 2.1, we obtain in the real representation of elements of $\mathcal{F}_h$

$$G^h(f+t)=G^h(f)+\nabla G^h(f).t+\frac{1}{2}t^T\mathrm{H}ess\, G^h(f)t+O(\|t\|^3_{\mathcal{F}_h})$$

for all $t\in\mathcal{F}^1_h$. If f solves (2.2) and $\|f+t\|_{\mathcal{F}_h}=\|f\|=1$, one obtains, while noting that the real gradient is equal to $2\lambda f$,

$$G^h(f+t)=G^h(f)+\frac{1}{2}t^T\left[\mathrm{H}ess\, G^h(f)-2\lambda\,\mathrm{Id}\right]t+O(\|t\|^3_{\mathcal{F}_h})\,.$$

By Proposition 2.3 the operator $P_\perp(\mathrm{H}ess\, f-2\lambda)P_\perp$ is a bounded from below self-adjoint operator with a compact resolvent. If the proposition is not true, it admits a negative eigenvalue $-\alpha_0<0$ with a normalized eigenvector φ. This eigenvector solves the equation

$$\mathrm{H}ess\, G^h(f)\varphi=(2\lambda-\alpha_0)\varphi+\alpha_1 f,\quad \alpha_1\in\mathbb{R}\,.$$

It implies $\varphi\in\mathcal{F}^2_h\cap f^\perp$ while the Euler-Lagrange (2.2) equation also gives $f\in\mathcal{F}^2_h$. We take

$$t=t(\delta)=\|f+\delta\varphi\|^{-1}(f+\delta\varphi)-f=\delta\varphi+((1+\delta^2)^{-1}-1)f+\left((1+\delta^2)^{-1}-1\right)\delta\varphi$$

and we obtain

$$G^h(f+t(\delta))=G^h(f)-\frac{\alpha_0}{2}\delta^2+O(\delta^3)$$

with $\|f+t(\delta)\|=1$, which is impossible. $\square$

3 The Hamiltonian flow

The Hamilton equations associated with the energy $G^h(f)$ in the Bargmann space $\mathcal{F}_h$ simply reads

$$i\partial_t f = 2\nabla_{\overline{f}} G^h(f) = 2(N_h + h)f + 2Na\Omega_h^2 \Pi_h(e^{-\frac{|z|^2}{h}} |f|^2) f\,. \tag{3.1}$$

We recall that the symplectic structure is given by

$$\sigma(f_1, f_2) = -\mathcal{I}\mathrm{m}\, \langle f_1 \mid f_2 \rangle_{\mathcal{F}_h}$$

according to Subsection 2.2.
We first refer to the Appendix for some notations and results about the nonlinear Hamiltonian flow on $\mathcal{F}_h$. Then, we introduce a modified energy

$$G^h_{\Phi_0,\Phi_1}(f) = G^h(f) + \Phi_0(\|f\|^2_{\mathcal{F}_h}) + \Phi_1(\langle f \mid N_h f\rangle_{\mathcal{F}_h})\,.$$

which allows to handle easily the restriction to the sphere $\left\{\|f\|_{\mathcal{F}_h} = 1\right\}$ and the degeneracy of the minimization problem due to the rotational symmetry. Finally, we tackle the linearization problem: Owing to Proposition 2.5 and results of Appendix A, we are able to select properly the modifier Φ_0 and Φ_1 so that the linearized Hamiltonian has a discrete purely imaginary spectrum $(i\mu_n)_{n\in\mathbb{Z}^*}$ with $\mu_{-n} = -\mu_n$ and $\lim_{n\to\infty} |\mu_n| = +\infty$.

3.1 The Cauchy problem

We check here that the Hamiltonian flow associated with (3.1) is well defined and admits two preserved quantities. We consider the Cauchy problem

$$\left\{\begin{array}{l} i\partial_t f = 2(N_h + h)f + 2Na\Omega_h^2 \Pi_h(e^{-\frac{|z|^2}{h}} |f|^2) f \\ f(t=0) = f_0\,. \end{array}\right. \tag{3.2}$$

Proposition 3.1. *For any $f_0 \in \mathcal{F}_h^2$, the Cauchy problem (3.2) admits a unique solution in $\mathcal{C}^0(\mathbb{R};\mathcal{F}_h^2) \cap \mathcal{C}^1(\mathbb{R};\mathcal{F}_h)$.*
The flow $\phi(t)$ defined by $\phi(t)f_0 = f(t)$ admits a unique continuous extension to $\mathcal{F}_h$, so that $\phi(t)f_0 \in \mathcal{C}^0(\mathbb{R};\mathcal{F}_h)$ for all $f_0 \in \mathcal{F}_h$.
This flow admits three preserved quantities. By setting $f(t) = \phi(t)f_0$, they are given by:

$$\begin{aligned}
&\forall f_0 \in \mathcal{F}_h, \forall t \in \mathbb{R}, \quad \|f(t)\|^2_{\mathcal{F}_h} = \|f_0\|^2_{\mathcal{F}_h}\,,\\
&\forall f_0 \in \mathcal{F}_h^2, \forall t \in \mathbb{R}, \quad G^h(f(t)) = G^h(f_0)\,,\\
&\forall f_0 \in \mathcal{F}_h^2, \forall t \in \mathbb{R}, \quad \langle f(t) \mid N_h f(t)\rangle_{\mathcal{F}_h} = \langle f_0 \mid N_h f_0\rangle_{\mathcal{F}_h}\,.
\end{aligned}$$

Proof: We use the results of Proposition A.8 in Appendix A. We simply specify here the corresponding notations. The Kaehler space $\mathcal{H}$ is the underlying real vector space of $\mathcal{F}_h$. An element $f = f_R + if_I$ of $\mathcal{F}_h$ is identified with $\begin{pmatrix} f_R \\ f_I \end{pmatrix}$ according to

Subsection 2.2. The real scalar product and the symplectic form on $\mathcal{H}$ are the ones defined in Subsection 2.2, while the involution J is the multiplication by i in $\mathcal{F}_h$ corresponding to the matrix $\begin{pmatrix} 0 & -\mathrm{Id} \\ \mathrm{Id} & 0 \end{pmatrix}$. The complexified space $\mathcal{H}_{\mathbb{C}}$ is simply $\mathcal{F}_h \oplus \mathcal{F}_h$ where a new multiplication by i is authorized componentwise. The operator A is $2(N_h+h)$ in $\mathcal{F}_h$, which corresponds $\begin{pmatrix} 2N_h+2h & 0 \\ 0 & 2N_h+2h \end{pmatrix}$ in the real space $\mathcal{H} \sim \mathcal{F}_h$ or its complexification $\mathcal{H}_{\mathbb{C}} = \mathcal{F}_h \oplus \mathcal{F}_h$. It is real, $A\left(D(A) \cap \mathcal{H}\right) \subset \mathcal{H}$, it has a compact resolvent and it commutes with J. The function $\mathfrak{h}(f)$ is the nonlinear part of $G^h(f)$:

$$
\begin{aligned}
\mathfrak{h}(f) &= \frac{Na\Omega_h^2}{2} \int_{\mathbb{C}} |f(z)|^4 e^{-\frac{2|z|^2}{h}} \; L(dz) \\
&= \frac{Na\Omega_h^2}{2} \int_{\mathbb{C}} \left(f_R(\overline{z}) - i f_I(\overline{z})\right)^2 \left(f_R(z) + i f_I(z)\right) e^{-\frac{2|z|^2}{h}} \; L(dz) \\
&= \frac{Na\Omega_h^2}{2} \int_{\mathbb{C}} \left(\overline{f_R}(\overline{z}) - i \; \overline{f_I}(\overline{z})\right)^2 \left(f_R(z) + i f_I(z)\right) e^{-\frac{2|z|^2}{h}} \; L(dz)\,.
\end{aligned}
$$

Its expression in terms of $\begin{pmatrix} f_R \\ f_I \end{pmatrix}$ and the continuity property of Lemma 2.1 show that it is real analytic in $\mathcal{H}$. The last expression, due to $\overline{f_R} = f_R$ and $\overline{f_I} = f_I$ when $f \in \mathcal{F}_h$, allows its extension as a real valued, real analytic function, with $\mathfrak{h}(e^{\alpha J} f) = \mathfrak{h}(f)$, to the complexified space $\mathcal{H}_{\mathbb{C}} = \mathcal{F}_h \oplus \mathcal{F}_h$ as it is required in Hypothesis A.2. The relation $\mathfrak{h}(e^{i\alpha N_h} f) = \mathfrak{h}(f)$ for $\alpha \in \mathbb{R}$ and $f \in \mathcal{F}_h$, which is the invariance of the above functional with respect to rotations, provides the gauge invariance required in Proposition A.8. $\square$

Remark 3.2. *Although we are working with an infinite dimensional system, the conservation of $\|f(t)\|_{\mathcal{F}_h}$ and $\langle f(t) \,|\, N_h f(t)\rangle_{\mathcal{F}_h}$ can be viewed as a consequence of Noether's Theorem (see [AbMa][Arn]). These quantities are associated with the invariance with respect to the multiplication by a phase factor $f \to e^{i\alpha} f$ and with respect to the rotations $f \to e^{i\alpha N_h} f$, $\alpha \in \mathbb{R}$, of the energy functional G^h.*

3.2 A modified Hamiltonian

Modifying the energy functional with the help of preserved quantities in order to study the stability of equilibrium in Hamiltonian systems is a standard process. This can be viewed for our specific Hamiltonian dynamics as a variation of the Casimir functional method. We refer for example to [HMRW] where many applications are discussed.
Here a modified Hamiltonian is introduced for two reasons:

1) We are interested in the stability of a constrained minimum.

2) The minimization problem is degenerate due to the rotational invariance.

We verify at the end of this paragraph that this modification of the energy functional makes sense and allows to catch relevant information on the dynamics.

First of all, we note that a solution f to the Euler-Lagrange equation (2.2) with Lagrange multiplier λ, is nothing but a critical point of the functional

$$G^h_{\Phi_0}(\varphi) = G^h(\varphi) + \Phi_0(\|\varphi\|^2_{\mathcal{F}_h})\,,$$

where Φ_0 is $\mathcal{C}^2$ function on $\mathbb{R}_+$ such that $\Phi_0'(1) = -\lambda$. Due to the conservation of $\|f(t)\|_{\mathcal{F}_h}$ by the Hamiltonian flow $\phi(t)$ associated with G^h, the new dynamics is well understood in terms of classical solutions: for $f_0 \in \mathcal{F}^2_h$, the Cauchy problem

$$\begin{cases} i\partial_t g = 2\partial_{\overline{g}} G^h_{\Phi_0}(g) \\ g(t=0) = f_0\,. \end{cases} \tag{3.3}$$

has a unique classical solution $g \in \mathcal{C}^1(\mathbb{R};\mathcal{F}_h) \cap \mathcal{C}^0(\mathbb{R};\mathcal{F}^2_h)$. It is equal to

$$g(t) = e^{-2it\Phi_0'(\|f_0\|^2_{\mathcal{F}_h})}\phi(t)f_0\,.$$

Hence a solution f to the Euler-Lagrange equation (2.2) with Lagrange multiplier λ, is transformed by taking $\Phi_0'(1) = -\lambda$ into an (unconstrained) equilibrium for the new Hamiltonian dynamics. Moreover the new dynamics for all other initial data is obtained after applying an elementary change of phase.

The second modification will help to get rid of the degeneracy problem due to the rotational invariance.

Definition 3.3. *Let $f \in \mathcal{F}^2_h$ be a solution to the Euler-Lagrange equation (2.2) with Lagrange multiplier $\lambda \in \mathbb{R}$ and $\|f\|_{\mathcal{F}_h} = 1$. The functionals $\varphi \mapsto \Phi_0(\|\varphi\|^2_{\mathcal{F}_h})$ and $\varphi \mapsto \Phi_1(\langle \varphi \,|\, N_h\varphi\rangle_{\mathcal{F}_h})$ are said to be adapted to (f,λ) if*

- *Φ_0 and Φ_1 are $\mathcal{C}^2$ real-valued functions on $[0,+\infty)$.*
- *$\Phi_0'(1) = -\lambda$ ($\|f\|_{\mathcal{F}_h} = 1$) and $\Phi_1'(\langle f \,|\, N_h f\rangle_{\mathcal{F}_h}) = 0$.*

In such a case, the adapted energy is defined by

$$G^h_{\Phi_0,\Phi_1}(\varphi) = G^h(\varphi) + \Phi_0(\|\varphi\|^2_{\mathcal{F}_h}) + \Phi_1(\langle \varphi \,|\, N_h\varphi\rangle_{\mathcal{F}_h})\,.$$

Remark 3.4. *The condition $f \in \mathcal{F}^2_h$ is not a restriction because an element $f \in \mathcal{F}_h$ which solves the Euler-Lagrange equation (2.2) necessarily belongs to $\mathcal{F}^2_h$.*

The same argument as above leads to:

Proposition 3.5. *Let f be a solution to (2.2) with Lagrange multiplier λ. Let $\Phi_0(\|\varphi\|^2_{\mathcal{F}_h})$ and $\Phi_1(\langle \varphi \,|\, N_h\varphi\rangle_{\mathcal{F}_h})$ be adapted to the pair (f,λ) according to Definition 3.3. Then for any $f_0 \in \mathcal{F}^2_h$, the function*

$$\varphi(z,t) = e^{-2it\Phi_0'(\|f_0\|^2_{\mathcal{F}_h})}[\phi(t)f_0](e^{-2iht\Phi_1'(\langle f_0 \,|\, N_h f_0\rangle_{\mathcal{F}_h})}z)$$

is the unique classical solution ($\varphi \in \mathcal{C}^0(\mathbb{R};\mathcal{F}^2_h) \cap \mathcal{C}^1(\mathbb{R};\mathcal{F}_h)$) of the Cauchy problem

$$\begin{cases} i\partial_t \varphi = 2\partial_{\overline{\varphi}} G^h_{\Phi_0,\Phi_1}(\varphi) \\ \varphi(t=0) = f_0\,. \end{cases} \tag{3.4}$$

Proof: It is sufficient to write

$$\partial_{\overline{\varphi}} G^h_{\Phi_0,\Phi_1}(\varphi) = \partial_{\overline{\varphi}} G^h(\varphi) + \Phi_0'(\|\varphi\|^2_{\mathcal{F}_h})\varphi + \Phi_1'(\langle \varphi \,|\, N_h\varphi\rangle_{\mathcal{F}_h}) zh\partial_z\varphi\,.$$

If φ is a classical solution to (3.4) then

$$e^{2i\int_0^s \Phi_0'(\|\varphi(s)\|^2_{\mathcal{F}_h})\ ds}\varphi\big(e^{2ih\int_0^s \Phi_1'\left(\langle\varphi\,|\,N_h\varphi\rangle_{\mathcal{F}_h}\right)\ ds} z\big)$$

is a classical solution to (3.2). Proposition 3.1 yields the result. □

The modification of the energy functional does not change the dynamics of the solution f to the Euler-Lagrange equation (2.2). For other initial data, it is changed by a multiplication by a phase factor and by the action of a uniform solid rotation. These additional time dependence are slow when the initial data f_0 is close to the critical point f. In the spectral stability analysis which follows, this means that we consider the stability up to the multiplication by a phase factor (which does not change the modulus of the wave function $|u|^2 = |f(z)|^2 e^{-\frac{|z|^2}{h}}$) and up to a uniform (and slow) solid rotation.

3.3 Linearized Hamiltonian

Here we consider a solution f to the minimization problem (1.4). Although it is a degenerate constrained minimization problem in infinite dimension, the introduction of a modified energy allows to recover the expected properties of the linearized Hamiltonian.

Theorem 3.6. *Assume that $f \in \mathcal{F}_h^1$ is a solution to the minimization problem (1.4) with Lagrange multiplier λ. Assume moreover that the functional $G^h_{\Phi_0,\Phi_1}$ is adapted to the pair (f, λ) according to Definition 3.3 and set $\alpha_0 = \Phi_0''(\|f\|^2_{\mathcal{F}_h})$ and $\alpha_1 = \Phi_1''(\langle f \,|\, N_h f\rangle_{\mathcal{F}_h})$. Then f is a spectrally stable equilibrium for the energy $G^h_{\Phi_0,\Phi_1}$ provided that*

$$\alpha_0 - \frac{1}{\alpha_1} \geq 2h - 2\lambda\,, \quad \alpha_1 > 0\,.$$

The spectrum $\sigma(-J\mathrm{H}ess\, G^h_{\Phi_0,\Phi_1}(f))$ is made of a discrete set of eigenvalues $(i\mu_n)_{n\in\mathbb{Z}^*}$ with finite multiplicity such that $\mu_n \in \mathbb{R}$, $\mu_{-n} = -\mu_n$ and $\lim_{n\to\infty}|\mu_n| = +\infty$.

According to [HMRW], the spectral stability simply says that the spectrum of the linearized Hamiltonian

$$\begin{pmatrix} 0 & \mathrm{Id} \\ -\mathrm{Id} & 0 \end{pmatrix} \mathrm{H}ess\, G^h_{\Phi_0,\Phi_1}(f) = -J\mathrm{H}ess\, G^h_{\Phi_0,\Phi_1}(f)$$

is purely imaginary. According to the notation of Appendix A, J denotes the matrix $\begin{pmatrix} 0 & -\mathrm{Id} \\ \mathrm{Id} & 0 \end{pmatrix}$ in the real symplectic space $\mathcal{H} \sim \mathcal{F}_h$. We recall that the spectrum of a linear Hamiltonian has two symmetries with respect to $\mathbb{R}$ and $i\mathbb{R}$. Note however that in the spectrally stable case, a pure imaginary spectrum does not mean that the Hamiltonian is anti-adjoint (see Appendix A).

Lemma 3.7. *With the same assumptions as in Theorem 3.6, the Hessian* $\mathrm{Hess}\, G^h_{\Phi_0,\Phi_1}(f)$ *equals*

$$\mathrm{H}ess\, G^h_{\Phi_0,\Phi_1}(f) = \mathrm{H}ess\, G^h(f) - 2\lambda\, \mathrm{Id} + 4\alpha_0 \begin{pmatrix} |f_R\rangle\langle f_R| & |f_R\rangle\langle f_I| \\ |f_I\rangle\langle f_R| & |f_I\rangle\langle f_I| \end{pmatrix}$$
$$+ 4\alpha_1 \begin{pmatrix} |N_h f_R\rangle\langle N_h f_R| & |N_h f_R\rangle\langle N_h f_I| \\ |N_h f_I\rangle\langle N_h f_R| & |N_h f_I\rangle\langle N_h f_I| \end{pmatrix}$$

with $\alpha_0 = \Phi_0''(\|f\|^2_{\mathcal{F}_h})$ *and* $\alpha_1 = \Phi_1''(\langle f\,|\,N_h f\rangle_{\mathcal{F}_h})$ *Except for the lower bound which now depends on* α_0 *and* α_1 *it shares the properties of* $\mathrm{Hess}\, G^h$ *stated in Proposition 2.3.*

Proof: A direct calculation leads to

$$\begin{aligned} \varphi^T \mathrm{H}ess\, \Phi_0\left(\|f\|^2_{\mathcal{F}_h}\right)\varphi &= 2\Phi_0'(\|f\|^2_{\mathcal{F}_h})\,\|\varphi\|^2_{\mathcal{F}_h} + \Phi_0''\left(\|f\|^2_{\mathcal{F}_h}\right) 4\left(\mathbb{R}\mathrm{e}\langle f\,|\,\varphi\rangle_{\mathcal{F}_h}\right)^2 \\ \varphi^T \mathrm{H}ess\, \Phi_1\left(\langle f\,|\,N_h f\rangle_{\mathcal{F}_h}\right)\varphi &= 2\Phi_1'(\langle f\,|\,N_h f\rangle_{\mathcal{F}_h})\,\langle \varphi\,|N_h \varphi\rangle_{\mathcal{F}_h} \\ &\quad + \Phi_1''\left(\langle f\,|\,N_h f\rangle_{\mathcal{F}_h}\right) 4\left(\mathbb{R}\mathrm{e}\langle N_h f\,|\,\varphi\rangle_{\mathcal{F}_h}\right)^2 \end{aligned}$$

We conclude with $\Phi_0'(\|f\|^2_{\mathcal{F}_h}) = -\lambda$, $\Phi_1'(\langle f\,|\,N_h f\rangle_{\mathcal{F}_h}) = 0$ and with the identification between $\varphi = \varphi_R + i\varphi_I$ with $\begin{pmatrix} \varphi_R \\ \varphi_I \end{pmatrix}$. $\square$

Proof of Theorem 3.6: We refer again to the general framework reviewed in Appendix A, namely Proposition A.5 with $A = 2N_h$ and $B = \mathrm{H}ess\, G^h_{\Phi_0,\Phi_1} - 2N_h$. The above expression for $\mathrm{H}ess\, G^h_{\Phi_0,\Phi_1}$ combined with Proposition 2.3 and the fact that $f \in \mathcal{F}^2_h = D(N_h)$, implies that B is a bounded real operator. Proposition A.5 states that the spectral stability can be deduced from

$$\forall \varphi \in \mathcal{F}^1_h, \quad \varphi^T \mathrm{H}ess\, G^h_{\Phi_0,\Phi_1}(f)\varphi \geq 0\,.$$

Any element of $\mathcal{F}^1_h$ can be written $\varphi + \delta f$ with $\varphi \in f^\perp$ (i.e. $\mathbb{R}\mathrm{e}\,\langle f, \varphi\rangle_{\mathcal{F}_h} = 0$) and $\delta \in \mathbb{R}$. We get

$$\begin{aligned} &(\varphi + \delta f)^T \mathrm{H}ess\, G^h_{\Phi_0,\Phi_1}(f)(\varphi + \delta f) = \\ &\quad \varphi^T(\mathrm{H}ess\, G^h(f) - 2\lambda)\varphi + 2\delta\varphi^T(\mathrm{H}ess\, G^h(f) - 2\lambda)f + \delta^2 f^T(\mathrm{H}ess\, G^h(f) - 2\lambda)f \\ &+4\alpha_0\delta^2\, \|f\|^4_{\mathcal{F}_h} + 4\alpha_1\left(\mathbb{R}\mathrm{e}\langle \varphi\,|\,N_h f\rangle_{\mathcal{F}_h}\right)^2 + 8\alpha_1\delta\langle f\,|\,N_h f\rangle_{\mathcal{F}_h}\, \mathbb{R}\mathrm{e}\langle \varphi\,|\,N_h f\rangle_{\mathcal{F}_h} + 4\alpha_1\delta^2\langle f\,|\,N_h f\rangle^2_{\mathcal{F}_h}\,. \end{aligned}$$

The first term $\varphi^T(\mathrm{H}ess\, G^h(f) - 2\lambda)\varphi$ is non negative according to Proposition 2.5. Since λ is real and $\varphi \in f^\perp$ the scalar products $\varphi^T \lambda f$ vanish. Proposition 2.3 (it is shorter to reproduce the calculation of G_2 in its proof) leads to

$$\begin{aligned} \varphi^T(\mathrm{H}ess\, G^h(f) - 2\lambda)f &= 2\,\mathbb{R}\mathrm{e}\langle \varphi\,|\,(N_h + h)f\rangle_{\mathcal{F}_h} + \\ &\quad (4+2)Na\Omega_h\, \mathbb{R}\mathrm{e}\langle \varphi\,|\,\Pi_h\left(e^{-\frac{|z|^2}{h}}\,|f|^2\, f\right)\rangle_{\mathcal{F}_h} - 2\lambda\,\mathbb{R}\mathrm{e}\langle \varphi\,|\,f\rangle_{\mathcal{F}_h} \end{aligned}$$

Then the Euler-Lagrange equation (2.2) implies for $\varphi \in f^{\perp}$

$$2\delta\varphi^T(\mathrm{H}ess\, G^h(f) - 2\lambda)f = -8\delta\,\mathbb{R}\mathrm{e}\langle\varphi\,|\,(N_h + h - \lambda)f\rangle_{\mathcal{F}_h} = -8\delta\,\mathbb{R}\mathrm{e}\langle\varphi\,|\,N_h f\rangle_{\mathcal{F}_h}$$

and

$$\delta^2 f^T(\mathrm{H}ess\, G^h(f) - 2\lambda)f = 8\delta^2(\lambda - h) - 8\delta^2\langle f\,|\,N_h f\rangle_{\mathcal{F}_h}\,.$$

Adding all the terms leads to

$$\begin{aligned}
&(\varphi + \delta f)^T\mathrm{H}ess\, G^h_{\Phi_0,\Phi_1}(f)(\varphi + \delta f) \geq \\
&\quad \geq -8\delta\,\mathbb{R}\mathrm{e}\langle\varphi\,|\,N_h f\rangle_{\mathcal{F}_h} + 8\delta^2(\lambda - h) - 8\delta^2\langle f\,|\,N_h f\rangle_{\mathcal{F}_h} + 4\alpha_0\delta^2 \\
&\qquad\quad + 4\alpha_1(\mathbb{R}\mathrm{e}\langle\varphi\,|\,N_h f\rangle_{\mathcal{F}_h})^2 + 8\alpha_1\delta\langle f\,|\,N_h f\rangle_{\mathcal{F}_h}\,\mathbb{R}\mathrm{e}\langle\varphi\,|\,N_h f\rangle_{\mathcal{F}_h} + 4\alpha_1\delta^2\langle f\,|\,N_h f\rangle^2_{\mathcal{F}_h} \\
&\quad \geq 4\delta^2(2\lambda - 2h + \alpha_0) \\
&\qquad\quad + 4\alpha_1\delta^2\left[r^2 + 2\left(\langle f\,|\,N_h f\rangle_{\mathcal{F}_h} - \frac{1}{\alpha_1}\right)r + \langle f\,|\,N_h f\rangle_{\mathcal{F}_h}\left(\langle f\,|\,N_h f\rangle_{\mathcal{F}_h} - \frac{2}{\alpha_1}\right)\right] \\
&\quad \geq 4\delta^2(2\lambda - 2h + \alpha_0) + 4\alpha_1\delta^2\left[\left(r + \langle f\,|\,N_h f\rangle_{\mathcal{F}_h} - \frac{1}{\alpha_1}\right)^2 - \frac{1}{\alpha_1^2}\right]
\end{aligned}$$

by setting $r = \frac{\mathbb{R}\mathrm{e}\langle\varphi\,|\,N_h f\rangle_{\mathcal{F}_h}}{\delta}$ and for $\alpha_1 \neq 0$. Finally the last right-hand side is non negative for $\alpha_1 > 0$ and $\alpha_0 - \alpha_1^{-1} - 2h + 2\lambda > 0$. $\square$

4 Approximation by a finite dimensional problem

The approximation of the optimization problem (1.4) by finite dimensional ones, that is $\mathcal{F}_h$ is replaced by a set of polynomials with bounded degree, was studied in [ABN2]. Here we complete this information by showing that such a convergence result can be extended to the linearized Hamiltonian in the norm resolvent sense. We end this section by recalling that a more quantitative estimate of the convergence of spectral elements, in such a discretization process, is a real issue because the linearized Hamiltonian $-J\mathrm{H}ess\, G^h(f)$ is not anti-adjoint.

4.1 Preliminaries

For $K \in \mathbb{N}$, $\mathbb{C}_K[z]$ denotes the set of polynomials with degree smaller than or equal to K. Since $(c_{n,h}z^n)_{n\in\mathbb{N}}$, $c_{nh} = \frac{1}{(\pi h)^{1/2}h^{n/2}\sqrt{n!}}$, is an orthonormal spectral basis for N_h with $N_h z^n = hnz^n$, the orthogonal projection $\Pi_{h,K}$ onto $\mathbb{C}_K[z]$ coincides with the orthogonal spectral projection:

$$\Pi_{h,K} = 1_{[0,hK]}(N_h)\,.$$

We shall use the notation $\Pi'_{h,K}$ for the imbedding from $\mathbb{C}_K[z]$ into $\mathcal{F}_h$:

$$\Pi_{h,K} \circ \Pi'_{h,K} = \mathrm{Id}_{\mathbb{C}_K[z]} \qquad \Pi'_{h,K} \circ \Pi_{h,K} = \Pi_{h,K}\,. \tag{4.1}$$

We introduce the reduced minimum of the finite dimensional optimization problem:

$$e^h_{LLL,K} = \min_{P\in\mathbb{C}_K[z],\|P\|_{\mathcal{F}_h}=1} G^h(P)\ . \tag{4.2}$$

Theorem 4.1. ***1)*** *The minima e^h_{LLL} and $e^h_{LLL,K}$ satisfy*

$$\forall K\in\mathbb{N}\cap(h^{-1}C_2(h),+\infty),\quad 0<e^h_{LLL,K}-e^h_{LLL}\leq\frac{C_2(h)^2+C_2(h)^3}{(1-C_2(h)(hK)^{-1})^4}(hK)^{-1}$$

where $C_2(h)=\frac{8\Omega_h}{3\pi}\sqrt{\frac{2bNa}{h}}+o_{Na}(h^{-1/2})$ does not depend on K.
If f solves the minimization problem (1.4) then the sequence $(f_K)_{K\in\mathbb{N}}$ defined by $f_K=\|\Pi_{h,K}f\|^{-1}\,\Pi_{h,K}f$, which satisfies $f_K\in\mathbb{C}_K[z]$ is a minimizing sequence for (1.4).
2) *If for any $K\in\mathbb{N}$, $P_K\in\mathbb{C}_K[z]$ denotes any solution to (4.2) then the sequence $(P_K)_{K\in\mathbb{N}}$ is a minimizing sequence for (1.4). Its accumulation points for the $\|\ \|_{\mathcal{F}_h}$ topology are solutions of (1.4). Moreover if a subsequence $(P_{K_n})_{n\in\mathbb{N}}$ converges to f in $\mathcal{F}_h$ then the convergence also holds in $\mathcal{F}^2_h$ according to:*

$$\lim_{n\to\infty}\|f-P_K\|_{\mathcal{F}_h}+\|N_h(f-P_{K_n})\|_{\mathcal{F}_h}=0\,.$$

4.2 Convergence of the linearized Hamiltonian

We now consider the question of the convergence of the linearized Hamiltonians associated with the functional $G^h_{\Phi_0,\Phi_1}$. We forget the term related to the gradient of the functionals since in the end it will be applied with critical points. The linearized Hamiltonian at a point $\varphi\in\mathcal{F}_h$ is defined as

$$H_\infty(\varphi):=-J\mathrm{H}ess\,G^h_{\Phi_0,\Phi_1}(\varphi)$$

with $J=\begin{pmatrix}0&-\mathrm{Id}\\ \mathrm{Id}&0\end{pmatrix}=\oplus_{n\in\mathbb{N}}\begin{pmatrix}0&-1\\1&0\end{pmatrix}$ in $\mathcal{F}_h\oplus\mathcal{F}_h=\oplus_{n\in\mathbb{N}}(\mathbb{C}z^n\oplus\mathbb{C}z^n)$. We keep the notation $\Pi_{h,K}$ for the diagonal operator

$$\Pi_{h,K}:=\begin{pmatrix}\Pi_{h,K}&0\\0&\Pi_{h,K}\end{pmatrix}\quad\text{in }\mathcal{F}_h\oplus\mathcal{F}_h\,.$$

Due to the commutation $\Pi_{h,K}J=J\Pi_{h,K}$ the restricted linearized Hamiltonian at a point of $G^h_{\Phi_0,\Phi_1}\big|_{\mathbb{C}_K[z]}$ equals

$$H_K(\varphi_K)=-\Pi_{h,K}\left(J\mathrm{H}ess\,G^h_{\Phi_0,\Phi_1}(\varphi_K)\right)\Pi'_{h,K}=-J\Pi_{h,K}\left(\mathrm{H}ess\,G^h_{\Phi_0,\Phi_1}(\varphi_K)\right)\Pi'_{h,K}\,.$$

For any holomorphic function θ in an open subset $\omega\subset\mathbb{C}$ and any <u>compact</u> regular contour $\gamma\subset\omega$ which does not meet the spectrum $\sigma(H_\infty(\varphi))$ the holomorphic functional calculus provides the operators

$$\theta_\gamma(H_\infty(\varphi))=\frac{1}{2\pi i}\oint_\gamma\theta(z)(z-H_\infty(\varphi))^{-1}\,dz \tag{4.3}$$

with a corresponding definition for $\theta_\gamma(H_K(\varphi_K))$.

Theorem 4.2. *With the notations of Theorem 4.1, let $(P_{K_n})_{n\in\mathbb{N}}$ denote a converging subsequence of solutions of (4.2) with $K = K_n$, and let f denote the limit $f = \lim_{n\to\infty} P_{K_n}$ which is a solution to (1.4). Then for all $z \in \mathbb{C}\setminus\sigma(H_\infty(f))$, the convergence*

$$\lim_{n\to\infty} \Pi'_{h,K_n}(z\,\mathrm{Id}_{\mathbb{C}_{K_n}[z]\oplus\mathbb{C}_{K_n}[z]} - H_{K_n}(P_{K_n}))^{-1}\Pi_{h,K_n} = (z - H_\infty(f))^{-1}$$

holds in the norm topology. Hence for any pair (γ,θ) (see (4.3)) such that $\gamma\cap\sigma(H_\infty(f)) = \emptyset$ the convergence

$$\lim_{n\to\infty} \Pi'_{h,K_n}\theta_\gamma(H_{K_n}(P_{K_n}))\Pi_{h,K_n} = \theta_\gamma(H_\infty(f))$$

holds in the norm topology.

We start with a lemma derived after the introduction of a Grushin problem (see [SjZw] and references therein), a more flexible variation of the Feshbach method (see [DeJa] and references therein).

Lemma 4.3. *In a complex Hilbert space $(\mathcal{H}_\mathbb{C}, \langle . \,, . \rangle)$, let A be a self-adjoint operator with domain $D(A)$ and with a compact resolvent. Let $(\alpha_n)_{n\in\mathbb{N}}$ be a sequence of complex numbers such that $\lim_{n\to\infty}\alpha_n = 1$. Let $(B_n)_{n\in\mathbb{N}}$ be a sequence of bounded operators with limit B in the norm topology as $n\to\infty$: $\lim_{n\to\infty}\|B_n - B\| = 0$. Let Π_n be the spectral projection $1_{[-T_n,T_n]}(A)$ with the assumption $\lim_{n\to\infty} T_n = +\infty$. The imbedding $\mathrm{Ran}\,\Pi_n \to \mathcal{H}$ is denoted by Π'_n according to (4.1). Then the limit*

$$\lim_{n\to\infty} \Pi'_n(z\,\mathrm{Id}_{\mathrm{Ran}\,\Pi_n} - \Pi_n(\alpha_n A + B_n)\Pi'_n)^{-1}\Pi_n = (z - (A+B))^{-1}$$

holds in the norm topology for all $z \in \mathbb{C}\setminus\sigma(A+B)$.

Proof: **1)** We first consider the case $\alpha_n = 1$ for all $n \in \mathbb{N}$. We set

$$\beta = \sup\left\{\|B_n\|\,,\ n\in\mathbb{N}\right\}\cup\left\{\|B\|\right\}\,.$$

For $z \in \mathbb{C}$, we set $A_{nz} = z - (A + B_n) : D(A) \to \mathcal{H}$. After the decomposition $\mathcal{H} = \mathrm{Ran}\,\Pi_n \oplus \mathrm{Ran}(1-\Pi_n)$ and $D(A) = \mathrm{Ran}\,\Pi_n \oplus (D(A)\cap\mathrm{Ran}(1-\Pi_n))$, it is written:

$$A_{nz} = \begin{pmatrix} A_{nz}^{nn} & A_{nz}^{n\bar{n}} \\ A_{nz}^{\bar{n}n} & A_{nz}^{\bar{n}\bar{n}} \end{pmatrix} = \begin{pmatrix} A_{nz}^{nn} & -B_n^{n\bar{n}} \\ -B_n^{\bar{n}n} & A_{nz}^{\bar{n}\bar{n}} \end{pmatrix}$$

with $X^{nn} = \Pi_n X \Pi'_n$, $X^{n\bar{n}} = \Pi_n X(1-\Pi_n)'$, $X^{\bar{n}n} = (1-\Pi_n)X\Pi'_n$ and $X^{\bar{n}\bar{n}} = (1-\Pi_n)X(1-\Pi_n)'$. Accordingly we use the notation $A_{\infty,z}$ for $z - (A+B)$ with for $n\in\mathbb{N}$ fixed the corresponding restrictions $A_{\infty,z}^{nn}$, $A_{\infty,z}^{n\bar{n}} = B^{n\bar{n}}$, $A_{\infty,z}^{\bar{n}n} = B^{\bar{n}n}$ and $A_{\infty,z}^{\bar{n}\bar{n}}$. We follow [SjZw] for the introduction of the Grushin problem and we set:

$$\mathcal{A}_{nz} = \begin{pmatrix} A_{nz} & R_-^n \\ R_+^n & 0 \end{pmatrix} = \begin{pmatrix} A_{nz}^{nn} & B_n^{n\bar{n}} & \mathrm{Id}_{\mathrm{Ran}\,\Pi_n} \\ B_n^{n\bar{n}} & A_{nz}^{\bar{n}\bar{n}} & 0 \\ \mathrm{Id}_{\mathrm{Ran}\,\Pi_n} & 0 & 0 \end{pmatrix} : D(A)\oplus\mathrm{Ran}\,\Pi_n \to \mathcal{H}\oplus\mathrm{Ran}\,\Pi_n$$

with

$$R_-^n = \begin{pmatrix} \mathrm{Id}_{\mathrm{Ran}\,\Pi_n} \\ 0 \end{pmatrix} \quad \text{and} \quad R_+^n = (\mathrm{Id}_{\mathrm{Ran}\,\Pi_n}, 0)\ .$$

The Schur complement formula says that if

$$\mathcal{A}_{nz}^{-1} = \begin{pmatrix} E^n & E_+^n \\ E_-^n & E_{-+}^n \end{pmatrix}$$

the operator A_{nz} is invertible if and only if E_{-+}^n is invertible with

$$A_{nz}^{-1} = E^n - E_+^n (E_{-+}^n)^{-1} E_-^n, \quad (E_{-+}^n)^{-1} = -R_-^n A_{nz}^{-1} R_+^n\,. \tag{4.4}$$

We now compute $\mathcal{A}_{nz}^{-1}$. First note that for any $z \in \mathbb{C}$ there exists $n(z) \in \mathbb{N}$ such that $A_{nz}^{\bar{n}\bar{n}}$ is invertible for $n \geq n(z)$. The second resolvent formula gives:

$$(A_{nz}^{\bar{n}\bar{n}})^{-1} = (z - (1-\Pi_n)(A+B_n)(1-\Pi_n)')^{-1} = \left[1 + (z - A^{\bar{n}\bar{n}})^{-1} B_n^{\bar{n}\bar{n}}\right]^{-1} (z - A^{\bar{n}\bar{n}})^{-1}$$

where the self-adjoint operator $A^{\bar{n}\bar{n}} = (1-\Pi_n)A(1-\Pi_n)'$ has a spectrum included in $\mathbb{R} \setminus [-T_n, T_n]$. This also implies for $n \geq n(z)$:

$$\left\| \left[1 + (z - A^{\bar{n}\bar{n}})^{-1} B_n^{\bar{n}\bar{n}}\right]^{-1} \right\| \leq 2 \quad \text{and} \quad \left\| (A_{nz}^{\bar{n}\bar{n}})^{-1} \right\| \leq \frac{2}{||z| - T_n|} \overset{n\to\infty}{\to} 0\,.$$

In the former calculation B_n can be replaced by B so that

$$\left\| (A_{nz}^{\bar{n}\bar{n}})^{-1} \right\| \leq \frac{2}{||z| - T_n|}\,, \qquad \left\| (A_{\infty z}^{\bar{n}\bar{n}})^{-1} \right\| \leq \frac{2}{||z| - T_n|} \tag{4.5}$$

hold for $n \geq n(z)$.
The inverse $\mathcal{A}_{nz}^{-1}$ is computed by Gauss elimination:

$$\mathcal{A}_{nz}^{-1} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & (A_{nz}^{\bar{n}\bar{n}})^{-1} & -(A_{nz}^{\bar{n}\bar{n}})^{-1} B_n^{\bar{n}n} \\ 1 & -B_n^{n\bar{n}} (A_{nz}^{\bar{n}\bar{n}})^{-1} & -A_{nz}^{nn} + B_n^{n\bar{n}} (A_{nz}^{\bar{n}\bar{n}})^{-1} B_n^{\bar{n}n} \end{pmatrix}$$

The Schur complement formula (4.4) yields:

$$\begin{aligned} A_{nz}^{-1} = {} & (1-\Pi_n)' (A_{nz}^{\bar{n}\bar{n}})^{-1} (1-\Pi_n) + \\ & \begin{pmatrix} 1 \\ -(A_{nz}^{\bar{n}\bar{n}})^{-1} B_n^{\bar{n}n} \end{pmatrix} \left(A_{nz}^{nn} - B_n^{n\bar{n}} (A_{nz}^{\bar{n}\bar{n}})^{-1} B_n^{\bar{n}n} \right)^{-1} \left(1, -B_n^{n\bar{n}} (A_{nz}^{\bar{n}\bar{n}})^{-1} \right) \end{aligned} \tag{4.6}$$

when

$$E_{-+}^n = A_{nz}^{nn} - B_n^{n\bar{n}} (A_{nz}^{\bar{n}\bar{n}})^{-1} B_n^{\bar{n}n}$$

is invertible.
When $z \in \mathbb{C} \setminus \sigma(A+B)$, $A_{\infty,z}$ is invertible and the Schur complement formula (4.4) applied with B_n replaced by B implies that the operator

$$\widetilde{E_{-+}^n} = A_{\infty z}^{nn} - B^{n\bar{n}} (A_{\infty z}^{\bar{n}\bar{n}})^{-1} B^{\bar{n}n}$$

is invertible with
$$\left\|\left(\widetilde{E^n_{-+}}\right)^{-1}\right\| = \left\|R^n_- A^{-1}_{\infty z} R^n_+\right\|$$
uniformly bounded for $n \geq n(z)$. The second inequality of (4.5) implies
$$\left\|A^{nn}_{\infty z} - \widetilde{E^n_{-+}}\right\| \leq \frac{2\beta^2}{||z| - T_n|}, \quad \text{for} \;\; n \geq n(z)$$
and a uniform bound for $\|(A^{nn}_{\infty z})^{-1}\|$ with respect to $n \geq n(z)$. Owing to the convergences
$$\begin{aligned} &\|A^{nn}_{nz} - A^{nn}_{\infty z}\| \leq \|B - B_n\| \overset{n\to\infty}{\to} 0 \\ \text{and} \qquad &\left\|E^n_{-+} - A^{nn}_{nz}\right\| \leq \left\|B^{n\bar{n}}_n \left(A^{\bar{n}\bar{n}}_{n,z}\right)^{-1} B^{\bar{n}n}_n\right\| \leq \frac{2\beta^2}{||z| - T_n|} \overset{n\to\infty}{\to} 0\,, \end{aligned}$$
the same is true for $\|(A^{nn}_{nz})^{-1}\|$ and $\left\|E^n_{-+}\right\|$ and we get
$$\left\|(E^n_{-+})^{-1} - (A^{nn}_{nz})^{-1}\right\| \leq C_z \left\|B^{n\bar{n}}_n \left(A^{\bar{n}\bar{n}}_{n,z}\right)^{-1} B^{\bar{n}n}_n\right\| \leq \frac{2C_z\beta^2}{||z| - T_n|} \overset{n\to\infty}{\to} 0\,. \qquad (4.7)$$
We infer from (4.5), (4.6) and (4.7) the estimate
$$\left\|A^{-1}_{nz} - \Pi'_n (A^{nn}_{nz})^{-1}\Pi_n\right\| \leq \frac{C'_z}{||z| - T_n|} \overset{n\to\infty}{\to} 0\,.$$
The second resolvent formula also gives
$$\left\|A^{-1}_{nz} - A^{-1}_{\infty z}\right\| = \left\|(z - A - B_n)^{-1} - (z - A - B)^{-1}\right\| \overset{n\to\infty}{\to} 0\,,$$
which yields the result for $\alpha_n = 1$.
2) For the general case, it is enough to write
$$(z - \Pi_n(\alpha_n A + B_n - \Pi'_n)^{-1} = \frac{1}{\alpha_n}(\frac{z}{\alpha_n} - \Pi_n(A + \frac{1}{\alpha_n}B_n)\Pi'_n)^{-1} = \frac{1}{\alpha_n}(z - \Pi_n(A + \widetilde{B_n})\Pi'_n)^{-1}$$
with $\widetilde{B_n} = \alpha_n^{-1}B_n + (1 - \alpha_n^{-1})\,\mathrm{Id}$ and to apply the result of Part 1). □

Proof of Theorem 4.2: we recall that
$$G^h_{\Phi_0,\Phi_1}(f) = G^h(f) + \Phi_0\left(\|f\|^2_{\mathcal{F}_h}\right) + \Phi_1(\langle f \mid N_h f\rangle_{\mathcal{F}_h})$$
and its Hessian at a point $f \in \mathcal{F}^{+2}_h$ equals according to Lemma 3.7 (without assuming $\Phi'_1(\langle f \mid N_h f\rangle_{\mathcal{F}_h}) = 0$):
$$\begin{aligned} \mathrm{H}ess\, G^h_{\Phi_0,\Phi_1}(f) = \mathrm{H}ess\, G^h(f) &- 2\Phi'_0(\|f\|^2_{\mathcal{F}_h})\,\mathrm{Id} - 2\Phi'_1(\langle f \mid N_h f\rangle_{\mathcal{F}_h})N_h \\ &+ 4\Phi''_0(\|f\|^2_{\mathcal{F}_h})\begin{pmatrix} |f_R\rangle\langle f_R| & |f_R\rangle\langle f_I| \\ |f_I\rangle\langle f_R| & |f_I\rangle\langle f_I| \end{pmatrix} \\ &+ 4\Phi''_1(\langle f \mid N_h f\rangle_{\mathcal{F}_h})\begin{pmatrix} |N_h f_R\rangle\langle N_h f_R| & |N_h f_R\rangle\langle N_h f_I| \\ |N_h f_I\rangle\langle N_h f_R| & |N_h f_I\rangle\langle N_h f_I| \end{pmatrix}. \end{aligned}$$

When f solves (1.4) and for well chosen Φ_0 and Φ_1, it writes:

$$\begin{aligned}
\mathrm{H}ess\, G^h_{\Phi_0,\Phi_1}(f) &= \mathrm{H}ess\, G^h(f) - 2\lambda\,\mathrm{Id} + 4\alpha_0 \begin{pmatrix} |f_R\rangle\langle f_R| & |f_R\rangle\langle f_I| \\ |f_I\rangle\langle f_R| & |f_I\rangle\langle f_I| \end{pmatrix} \\
&\qquad\qquad + 4\alpha_1 \begin{pmatrix} |N_h f_R\rangle\langle N_h f_R| & |N_h f_R\rangle\langle N_h f_I| \\ |N_h f_I\rangle\langle N_h f_R| & |N_h f_I\rangle\langle N_h f_I| \end{pmatrix} \\
&= 2\begin{pmatrix} N_h & 0 \\ 0 & N_h \end{pmatrix} + \widetilde{B}\,,
\end{aligned}$$

where $\widetilde{B} \in \mathcal{L}(\mathcal{F}_h \oplus \mathcal{F}_h)\,.$ Meanwhile we obtain for P_{K_n} (with $\lim_{n\to\infty} P_{K_n} = f$ in $\mathcal{F}^2_h$):

$$\begin{aligned}
\mathrm{H}ess\, G^h_{\Phi_0,\Phi_1}(P_{K_n}) &= \mathrm{H}ess\, G^h(P_{K_n}) - 2\Phi_0'(\|P_{K_n}\|^2_{\mathcal{F}_h})\,\mathrm{Id} - 2\Phi_1'(\langle P_{K_n} \mid N_h P_{K_n}\rangle_{\mathcal{F}_h}) N_h \\
&\qquad + 4\Phi_0''(\|P_{K_n}\|^2_{\mathcal{F}_h}) \begin{pmatrix} |P_{K_n,R}\rangle\langle P_{K_n,R}| & |P_{K_n,R}\rangle\langle P_{K_n,I}| \\ |P_{K_n,I}\rangle\langle P_{K_n,R}| & |P_{K_n,I}\rangle\langle P_{K_n,I}| \end{pmatrix} \\
&\quad + 4\Phi_1''(\langle P_{K_n} \mid N_h P_{K_n}\rangle_{\mathcal{F}_h}) \begin{pmatrix} |N_h P_{K_n,R}\rangle\langle N_h P_{K_n,R}| & |N_h P_{K_n,R}\rangle\langle N_h P_{K_n,I}| \\ |N_h P_{K_n,I}\rangle\langle N_h P_{K_n,R}| & |N_h P_{K_n,I}\rangle\langle N_h P_{K_n,I}| \end{pmatrix} \\
&= 2(1 - \Phi_1'(\langle P_{K_n} \mid N_h P_{K_n}\rangle_{\mathcal{F}_h})) \begin{pmatrix} N_h & 0 \\ 0 & N_h \end{pmatrix} + \widetilde{B_n}
\end{aligned}$$

with

$$\lim_{n\to\infty} \Phi_1'(\langle P_{K_n} \mid N_h P_{K_n}\rangle_{\mathcal{F}_h}) = 0, \qquad \lim_{n\to\infty} \left\|\widetilde{B_n} - \widetilde{B}\right\| = 0\,.$$

By recalling

$$H_\infty(f) = -J\mathrm{H}ess\, G^h_{\Phi_0,\Phi_1}(f) \qquad \text{and} \qquad H_\infty(P_{K_n}) = -J\mathrm{H}ess\, G^h_{\Phi_0,\Phi_1}(P_{K_n})$$

and by applying Lemma 4.3 with

$$\begin{aligned}
& A = -2iJ \begin{pmatrix} N_h & 0 \\ 0 & N_h \end{pmatrix} = \begin{pmatrix} 0 & 2iN_h \\ -2iN_h & 0 \end{pmatrix}, \\
& \alpha_n = (1 - \Phi_1'(\langle P_{K_n} \mid N_h P_{K_n}\rangle_{\mathcal{F}_h})) \\
& B = -iJ\widetilde{B}\,, \quad B_n = -iJ\widetilde{B_n} \\
\text{and} \quad & \Pi_n = \begin{pmatrix} \Pi_{h,K_n} & 0 \\ 0 & \Pi_{h,K_n} \end{pmatrix} = \Pi_{h,K_n}, \qquad T_n = 2hK_n\,,
\end{aligned}$$

one gets

$$\lim_{n\to\infty} \Pi'_{h,K_n}(z\,\mathrm{Id}_{\mathbb{C}_{K_n}[z]\oplus\mathbb{C}_{K_n}[z]} - \Pi_{h,K_n} H_\infty(P_{K_n})\Pi'_{h,K_n})^{-1}\Pi_{h,K_n} = (z - H_\infty(f))^{-1}$$

for all $z \in \mathbb{C} \setminus \sigma(H_\infty(f))\,.$ We conclude with

$$H_{K_n}(P_{K_n}) = \Pi_{h,K_n} H_\infty(P_{K_n})\Pi'_{h,K_n}\,.$$

Finally the convergence of the spectral elements $\Pi'_{h,K_n}\theta_\gamma(H_{K_n}(P_{K_n}))\Pi_{h,K_n}$ comes from the fact that all the convergence estimates are locally uniform in z for $h > 0$ fixed. $\square$

4.3 Remarks about the stability of spectral quantities

Contrary to Theorem 4.1, the results of Theorem 4.2 about the stability of spectral quantities does not provide any quantitative estimate. For a fixed not so small value of $h > 0$ and when only a fixed finite number of spectral elements are computed, such a quantitative estimate is not crucial. It becomes definitely an issue when $h > 0$ gets small or if one is interested in a large number of spectral elements. For example, the behaviour of the sequence $(i\mu_n)_{n\in\mathbb{Z}^*}$ of eigenvalues of the linearized Hamiltonian $-J\mathrm{H}ess\, G^h_{\Phi_0,\Phi_1}(f)$ stated in Theorem 3.6, $\lim_{n\to\infty}|\mu_n| = +\infty$, can be stated more accurately since the problem amounts to looking at a bounded perturbation of the harmonic oscillator quantum Hamiltonian. Nevertheless this behaviour seems difficult to recover in numerical simulations[3]

A very likely explanation is that the linearized Hamiltonian $-J\mathrm{H}ess\, G^h_{\Phi_0,\Phi_1}(f)$ is not anti-adjoint. Whatever the choices of the functions Φ_0 and Φ_1 are, the Hessian $\mathrm{H}ess\, G^h_{\Phi_0,\Phi_1}(f)$ is a finite rank perturbation of $\mathrm{H}ess\, G^h(f)$ according to Lemma 3.7. But the commutator $\left[J, \mathrm{H}ess\, G^h(f)\right]$ can be computed from (2.9) and equals

$$\begin{pmatrix} -2C & 2B \\ 2B & 2C \end{pmatrix}.$$

The operators B and C, defined in (2.11)(2.12), are non vanishing Hilbert-Schmidt operators but with infinite rank. Hence the linear Hamiltonian $-J\mathrm{H}ess\, G^h_{\Phi_0,\Phi_1}(f)$ is not anti-adjoint in spite of a purely imaginary spectrum.

The stability of the spectrum of non self-adjoint (or non normal) operators with respect to perturbations enters in the theory of pseudospectral estimates and it is known that there can be a big gap between the knowledge of the spectrum and a good control of resolvent estimates with dramatic consequences in numerical computations. Such an analysis for pseudo-differential operators has had a great development in the recent years and we refer the reader to [Tre][Dav1][Dav2][DSZ][Hag1][Hag2][HerNi][HelNi][Pra][Zwo]. In order to perform such an analysis of the linearized Hamiltonian $-J\mathrm{H}ess\, G^h(f)$, a better information on the minimizer f than the one provided in [AfBl][ABN1][ABN2] is necessary.

A Specific infinite dimensional Hamiltonian systems

Our aim is not here to give a complete account on infinite dimensional Hamiltonian systems. We refer the reader for example to [ChMa][Kuk][BHK] for a more general presentation or different points of view. We simply briefly point out the properties which are relevant to our problem.

We consider a separable Kaehler space $(\mathcal{H}, (.\,|\,.), \sigma)$: $(\mathcal{H}, (.\,|\,.))$ is a <u>real</u> Hilbert space while σ is a symplectic form compatible with $(.\,|\,.)$. We recall that the last condition means that there exists a continuous $\mathbb{R}$-linear (skew-adjoint) operator on $\mathcal{H}$ such that

[3] according to discussions with A. Aftalion and X. Blanc.

$J^2 = -1$ and

$$\sigma(X,Y) = -(JX \,|\, Y) = (X \,|\, JY)\,.$$

Before going further, it is useful to introduce the complexified Hilbert space $\mathcal{H}_{\mathbb{C}}$ with the scalar product

$$(f_1 + if_2 \,|\, g_1 + ig_2)_{\mathbb{C}} = (f_1 \,|\, g_1) + (f_2 \,|\, g_2) + i\,(f_1 \,|\, g_2) - i\,(g_1 \,|\, f_2)\ .$$

In this framework the operator J becomes a skew-adjoint bounded involution

$$J^* = -J, \qquad J^2 = -\operatorname{Id}$$

which differs from $i\operatorname{Id}$.

Remark A.1. *It is important to note here that the complexified Hilbert space $\mathcal{H}_{\mathbb{C}}$ has nothing to do with the natural complex structure associated with J. In fact, the complexified space has no relationship with the symplectic structure on $\mathcal{H}$. It is introduced only in order to provide the framework for spectral theory. More precisely, consider the example where $\mathcal{H} = \mathbb{R}^{2n} = \mathbb{R}^n_x \times \mathbb{R}^n_\xi$ is endowed with*

- *the scalar product:* $(X \,|\, X') = \begin{pmatrix} x \\ \xi \end{pmatrix} \cdot \begin{pmatrix} x' \\ \xi' \end{pmatrix} = xx' + \xi\xi'$
- *and the symplectic form:* $\sigma(X,X') = \xi x' - x\xi'$.

Let $J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$. *After the identification between $X \in \mathbb{R}^{2n}$ and $z = x + i\xi \in \mathbb{C}^n$, the real scalar product happens to be the real part of the complex scalar product $(X \,|\, X') = \operatorname{Re} \overline{z}.z'$ and the symplectic form the opposite of the imaginary part $\sigma(X,X') = -\mathcal{I}\mathrm{m}\, \overline{z}.z'$, while the operator J is translated into the multiplication by i. Instead, the complexified space $\mathcal{H}_{\mathbb{C}}$ equals $\mathbb{C}^{2n}$ and allows the action of* $J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ *and the componentwise multiplication by the complex scalar i.*
In the case of our analysis, the Kaehler space is the complex Hilbert space $\mathcal{F}_h$. We have, as a set, $\mathcal{H} = \mathcal{F}_h$, after the identification between $f = f_R + if_I \in \mathcal{F}_h$ and $\begin{pmatrix} f_R \\ f_I \end{pmatrix} \in \mathcal{H}$ *while $\mathcal{H}_{\mathbb{C}}$ equals $\mathcal{F}_h \oplus \mathcal{F}_h$.*
As in the study of second variations, some properties and symmetries of a linearized Hamiltonian are more obvious when working with the real structure (the complexification being added only in order to apply spectral theory).

The energy functional is given by

$$H(f) = \frac{1}{2}\,(f \,|\, Af)_{\mathbb{C}} + \frac{1}{2}\,(f \,|\, Bf)_{\mathbb{C}} + \mathfrak{h}(f), \quad \forall f \in D(A) \subset \mathcal{H}_{\mathbb{C}}$$

where the operators A, B and the nonlinear function $\mathfrak{h}$ satisfy the next assumptions:

Hypothesis A.2. • *The operator $(A, D(A))$ is a non negative self-adjoint operator on $\mathcal{H}_{\mathbb{C}}$, with a compact resolvent, which commutes with J and which is real: $A\left(D(A)\cap\mathcal{H}\right)\subset\mathcal{H}$.*

- *The operator B is a bounded real ($B\mathcal{H}\subset\mathcal{H}$) self-adjoint operator on $\mathcal{H}_{\mathbb{C}}$ (non necessarily commuting with J).*
- *The function $\mathfrak{h}:\mathcal{H}_{\mathbb{C}}\longmapsto\mathbb{R}$ is real analytic and satisfies the gauge invariance $\mathfrak{h}(e^{\alpha J}f)=\mathfrak{h}(f)$ for all $\alpha\in\mathbb{R}$ and all $f\in\mathcal{H}_{\mathbb{C}}$.*

The Hamilton equation can be written as

$$\begin{cases} \partial_t f = -J\nabla H(f) = -JAf - JBf - J\nabla\mathfrak{h}(f) \\ f(t=0) = f_0 \in \mathcal{H} \quad (\text{or } \in \mathcal{H}_{\mathbb{C}})\,. \end{cases} \tag{A.1}$$

where ∇ denotes the gradient with respect to the scalar product $(.\,|\,.)$ in the real case and the gradient with respect to the real scalar product $\mathbb{R}\mathrm{e}\,(.\,|\,.)_{\mathbb{C}}$ in the complex case. As usual an equilibrium is a critical point of H.

Proposition A.3. *Assume Hypothesis A.2. Then the initial value problem (A.1) admits a unique mild global solution for any $f_0\in\mathcal{H}_{\mathbb{C}}$. Moreover the flow defined by $f(t)=\Phi(t)f_0$ for $f_0\in\mathcal{H}_{\mathbb{C}}$ and $t\in\mathbb{R}$ satisfies*

$$\begin{aligned} &\forall f_0\in\mathcal{H},\forall t\in\mathbb{R},\quad \Phi(t)f_0\in\mathcal{H}\\ \textit{and}\quad &\forall f_0\in\mathcal{H}_{\mathbb{C}},\forall t\in\mathbb{R},\quad \|\Phi(t)f_0\|_{\mathcal{H}_{\mathbb{C}}} = e^{\|[B,J]\|t/2}\,\|f_0\|_{\mathcal{H}_{\mathbb{C}}}\,. \end{aligned}$$

Proof: **1) The linear case with $B=0$:** Since the operator A has a compact resolvent, commutes with the involution J and is real, it admits an orthonormal basis of real eigenvectors $\{\psi_n\in\mathcal{H},\ J\psi_n\in\mathcal{H},\ n\in\mathbb{N}\}$ with

$$A\psi_n=\lambda_n\psi_n \quad\text{and}\quad AJ\psi_n=\lambda_nJ\psi_n$$

so that $\lambda_n\in\mathbb{R}$ and $\lim_{n\to\infty}|\lambda_n|=+\infty$.

The operator $-iJA$ is self-adjoint with domain $D(A)$ and writes in $\mathcal{H}_{\mathbb{C}}=\oplus_{n\in\mathbb{N}}(\mathbb{C}\psi_n\oplus\mathbb{C}J\psi_n)$ as the block diagonal operator

$$-iJA=\oplus_{n\in\mathbb{N}}\begin{pmatrix} 0 & i\lambda_n\\ -i\lambda_n & 0\end{pmatrix}.$$

Hence the equation

$$i\partial_t f=-iJAf$$

is solved by the unitary strongly continuous group $\left(e^{-it(-iJA)}\right)_{t\in\mathbb{R}}=(e^{-tJA})_{t\in\mathbb{R}}$, which admits the explicit block diagonal expression

$$e^{-tJA}=\oplus_{n\in\mathbb{N}}\begin{pmatrix}\cos(t\lambda_n) & \sin(t\lambda_n)\\ -\sin(t\lambda_n) & \cos(t\lambda_n)\end{pmatrix}.$$

Hence this linear evolution preserves the $\mathcal{H}_{\mathbb{C}}$-norm, the domain $D(A)$ and reality.
2) Local existence for the nonlinear case: The Duhamel formula

$$f(t) = e^{-tJA} f_0 - \int_0^t e^{-(t-s)JA} J(Bf(s) + \nabla\mathfrak{h}(f(s)))\, ds\,.$$

and the analyticity assumption on $\mathfrak{h}$ allow to use the standard fixed point argument in $\mathcal{C}^0([0,T_{f_0}]\,;\mathcal{H}_{\mathbb{C}})$. The fixed point provides the real analyticity of $f(t)$ with respect to $f_0 \in \mathcal{H}_{\mathbb{C}}$. Finally, the uniqueness in $\mathcal{C}^0\,([0,T_{f_0}];\mathcal{H}_{\mathbb{C}})$ and the fact that the integral equation can be solved in $\mathcal{C}^0([0,T_{f_0}];\mathcal{H})$ ensures that $f(t) \in \mathcal{H}$ for all $t \in [0,T_{f_0}]$ as soon as $f_0 \in \mathcal{H}$.
3) Approximation with a bounded generator: In order to establish the preserved quantities, we approximate the linear operator by bounded ones. Let $A_\Lambda = 1_{[0,\Lambda]}(A)A$. By the spectral theorem, we get

$$\left\|(e^{-tJA_\Lambda} - e^{-tJA})f\right\|^2 \left\|(e^{-it(-iJA_\Lambda)} - e^{-it(-iJA)})f\right\|^2 = \int_\Lambda^\infty \left|1 - e^{-it\lambda}\right|^2\, d\mu_f(\lambda)$$

where $d\mu_f$ is the spectral measure of the given element $f \in \mathcal{F}_h$ with respect to the self-ajoint operator $-iJA$. Hence by dominated convergence we get:

$$\forall t \in \mathbb{R}, \quad \operatorname*{s-lim}_{\Lambda\to\infty} e^{-tJA_\Lambda} = e^{-tJA}\,.$$

We write the difference between the two integral equations:

$$\begin{aligned} & f_\Lambda(t) = e^{-tJA_\Lambda} f_0 - \int_0^t e^{-(t-s)JA_\Lambda} J(Bf_\Lambda(s) + \nabla\mathfrak{h}(f_\Lambda(s)))\, ds \\ \text{and} \qquad & f(t) = e^{-tJA} f_0 - \int_0^t e^{-(t-s)JA} J(Bf(s) + \nabla\mathfrak{h}(f(s)))\, ds \end{aligned}$$

as

$$\begin{aligned} f(t) - f_\Lambda(t) = \left(e^{-tJA} - e^{-tJA_\Lambda}\right) f_0 - \int_0^t \left(e^{-(t-s)JA} - e^{-(t-s)JA_\Lambda}\right) J(Bf(s) + \nabla\mathfrak{h}(f(s)))\, ds \\ - \int_0^t e^{-(t-s)JA_\Lambda} JB(f(s) - f_\Lambda(s))\, ds - \int_0^t e^{-(t-s)JA_\Lambda} J\left(\nabla\mathfrak{h}(f(s)) - \nabla\mathfrak{h}(f_\Lambda(s))\right)\, ds\,. \end{aligned}$$

For a fixed f_0 and a fixed $t \in [0,T_{f_0}]$, the analyticity assumption on $\mathfrak{h}$ and the fact that e^{-tJA} and e^{-tJA_Λ} are unitary operators, lead to

$$\|f - f_\Lambda\|^2 \le \varepsilon_{f_0}(\Lambda) + C_{f_0} \int_{0,t} \|f(s) - f_\Lambda(s)\|^2\, ds$$

with $\lim_{\Lambda\to\infty} \varepsilon_{f_0}(\Lambda) = 0$. By the Gronwall Lemma, we obtain for any $f_0 \in \mathcal{H}_{\mathbb{C}}$ the existence of T_{f_0} such that

$$\forall t \in [0,T_{f_0}], \quad \lim_{\Lambda\to\infty} \|f(t) - f_\Lambda(t)\| = 0\,.$$

4) Upper bound for the norm and global existence: According to the first step, we can reduce the analysis to the case where A is a bounded operator. Then the local in time mild solution is a classical solution for any $f_0 \in \mathcal{H}_{\mathbb{C}}$. We compute

$$\begin{aligned}\partial_t \|f\|^2 &= (\partial_t f \,|\, f)_{\mathbb{C}} + (f \,|\, \partial_t f)_{\mathbb{C}} = -2\,\mathrm{Re}\,(JAf + JBf + J\nabla\mathfrak{h}(f) \,|\, f)_{\mathbb{C}} \\ &= -2\,\mathrm{Re}\,(f \,|\, J\nabla\mathfrak{h}(f))_{\mathbb{C}} - (JBf \,|\, f)_{\mathbb{C}} + (f \,|\, JBf)_{\mathbb{C}} \\ &\leq -2\,\mathrm{Re}\,(f \,|\, J\nabla\mathfrak{h}(f))_{\mathbb{C}} + \|[J,B]\|\,\|f\|^2\end{aligned}$$

Here we differentiate the gauge invariance of $\mathfrak{h}$, $\mathfrak{h}(e^{\alpha J}f) = f$,:

$$0 = \frac{d}{d_\alpha}\mathfrak{h}(e^{\alpha J}f)\big|_{\alpha=0} = \mathrm{Re}\,(\nabla\mathfrak{h}(f) \,|\, Jf)_{\mathbb{C}}\ .$$

We have proved $\partial_t \|f\|^2 \leq \|[B,J]\|\,\|f\|^2$ when f solves (A.1) with $A \in \mathcal{L}(\mathcal{H}_{\mathbb{C}})$. The inequality $\|f(t)\| \leq e^{\|[B,J]\|t/E}\,\|f_0\|$ can be extended to the case of unbounded A according to step 3).
Finally this norm control provides the existence of a global in time solution, $T_{f_0} = +\infty$, for any $f_0 \in \mathcal{H}_{\mathbb{C}}$. □

We now consider the conservation of energy under the additional assumption that the flow $\Phi(t)$ preserves the domain $D(A)$. This will be checked in the proof of Proposition A.8 below. We refer to [ChMa] for a more general statement.

Proposition A.4. *Under Hypothesis A.2 and if the flow $\Phi(t)$ preserves the domain $D(A)$ in the sense that the solution f to (A.1) belongs to $\mathcal{C}^0(\mathbb{R}; D(A))$ when $f_0 \in D(A)$, then the equality*

$$H(f(t)) = H(\Phi(t)f_0) = H(f_0)$$

holds for any $t \in \mathbb{R}$ and any $f_0 \in D(A)$.

Proof: If $f \in \mathcal{C}^0(\mathbb{R}; D(A))$, then the mild solution to (A.1) is a strong solution, $f \in \mathcal{C}^1(\mathbb{R}; \mathcal{H}_{\mathbb{C}})$. Since the gradient of H equals $Af + Bf + \nabla\mathfrak{h}(f)$ we write:

$$\begin{aligned}&\partial_t H(f) = \mathrm{Re}\,(Af + Bf + \nabla\mathfrak{h}(f) \,|\, \partial_t f)_{\mathbb{C}} \\ &= -\,\mathrm{Re}\,((A+B)f \,|\, J(A+B)f)_{\mathbb{C}} - \mathrm{Re}\,((A+B)f \,|\, J\nabla\mathfrak{h}(f))_{\mathbb{C}} - \mathrm{Re}\,(\nabla\mathfrak{h}(f) \,|\, J(A+B)f)_{\mathbb{C}} \\ &\qquad - \mathrm{Re}\,(\nabla\mathfrak{h}(f) \,|\, J\nabla\mathfrak{h}(f))_{\mathbb{C}} = 0\,.\end{aligned}$$

□

We now give some applications in specific cases arising in our analysis.

Proposition A.5. *Under Hypothesis A.2 with $\mathfrak{h} = 0$, then the Hamiltonian vector $-J(A+B)$ defines a linear closed unbounded operator on $\mathcal{H}_{\mathbb{C}}$ with domain $D(-J(A+B)) = D(A)$. It has a compact resolvent and its spectrum has symmetries with respect to the two axes $\mathbb{R}$ and $i\mathbb{R}$.*
Moreover if the energy $H(f) = \frac{1}{2}(f \,|\, (A+B)f)$ is non negative for all $f \in D(A) \cap \mathcal{H}$ then $\sigma(-J(A+B)) \subset i\mathbb{R}$.

Remark A.6. *Note that although $\sigma(J(A+B)) \subset i\mathbb{R}$, the operator $J(A+B)$ is not anti-adjoint (even in finite dimension), except when J and $A+B$ commute, $[J,B]=0$. The finite dimensional version of the final result is a very specific case of the classification of quadratic Hamiltonian functions which is reviewed in [Arn]-Appendix 6.*
Especially when applying this Proposition, a good identification of the Kaehler structure on $\mathcal{H}$ and the two different complex structures on $\mathcal{H}_{\mathbb{C}}$ is useful.

Proof: Since the operator is a bounded perturbation of $-JA$, the first statements are standard (see [ReSi]). Concerning the symmetries of the spectrum, the following equivalences hold:

$$\begin{aligned}(\lambda \notin \sigma(-J(A+B))) &\Leftrightarrow ((-J(A+B)-\lambda) \text{ invertible}) \\ &\Leftrightarrow \left(J(-(A+B)J-\lambda)J^{-1} \text{ invertible}\right) \\ &\Leftrightarrow \left((-(A+B)J-\lambda)^* = (J(A+B)-\overline{\lambda}) \text{ invertible}\right) \\ &\Leftrightarrow \left(-\overline{\lambda} \notin \sigma(-J(A+B))\right)\end{aligned}$$

and provide the symmetry with respect to $i\mathbb{R}$. For the second symmetry, we introduce the conjugate $\overline{u}$ of any vector $u \in \mathcal{H}_{\mathbb{C}}$ as the symmetric vector with respect the real subspace $\mathcal{H}$. Since J, A and B are real operators, we obtain [4] for any $u \in \mathcal{H}$, $u \neq 0$,

$$(-J(A+B)u = \lambda u) \Leftrightarrow \left(-J(A+B)\overline{u} = \overline{\lambda}\overline{u}\right) .$$

Since $-J(A+B)$ has a compact resolvent, its spectrum is thus symmetric with respect to $\mathbb{R}$.
Finally, assume that the energy $H(f) = \frac{1}{2}(f \,|\, (A+B)f)$ is non negative for all $f \in D(A) \cap \mathcal{H}$. Since $(A+B, D(A))$ is self-adjoint on $\mathcal{H}_{\mathbb{C}}$, this means that $A+B$ is a non negative operator and we get

$$(H(u) = 0, \quad u \in \mathcal{H}_{\mathbb{C}}) \Leftrightarrow (u \in \operatorname{Ker}(A+B)) .$$

Let $\lambda \in \sigma(-J(A+B))$ be a non zero eigenvalue with eigenvector $u_0 \neq 0$. Since $u_0 \in D(A+B) = D(A)$, $u(t) = e^{-tJ(A+B)}u_0 \in \mathcal{C}^0(\mathbb{R}; D(A))$ and according to Proposition A.4, the energy is conserved:

$$\begin{aligned}e^{2\,\mathbb{R}\mathrm{e}\,\lambda t}\,(u_0 \,|\, (A+B)u_0)_{\mathbb{C}} &= \left(e^{\lambda t}u_0 \,|\, (A+B)e^{\lambda t}u_0\right)_{\mathbb{C}} = (u(t) \,|\, (A+B)u(t))_{\mathbb{C}} \\ &= (u_0 \,|\, (A+B)u_0)_{\mathbb{C}} .\end{aligned}$$

Since $\lambda \neq 0$, we get $u_0 \notin \operatorname{Ker}(A+B)$, $(u_0 \,|\, (A+B)u_0)_{\mathbb{C}} \neq 0$ and $\mathbb{R}\mathrm{e}\,\lambda = 0$. □

Proposition A.7. *Under Hypothesis A.2, a sufficient condition for an equilibrium to be spectrally stable, is that it is a local minimum.*

[4] Especially for this argument, it is preferable to forget the complex structure on $\mathcal{H}$ identifying J with the multiplication by i.

Proof: According to [HMRW], an equilibrium is spectrally stable when the spectrum of the linearized Hamiltonian is included in $i\mathbb{R}$. At a critical point f of H, the linearized Hamiltonian equals

$$-JA - JB - J\mathrm{H}ess\,\mathfrak{h}(f) = -J(A + B + \mathrm{H}ess\,\mathfrak{h}(f))\,.$$

If f is a minimum for H then $A + B + \mathrm{H}ess\,\mathfrak{h}(f)$ is non negative owing to the analyticity property of $\mathfrak{h}$:

$$H(f+\varphi) = \frac{1}{2}\left(\varphi\,|\,(A + B + \mathrm{H}ess\,\mathfrak{h}(f))\varphi\right) + O(\|\varphi\|^3)\,.$$

By replacing B by $B + \mathrm{H}ess\,\mathfrak{h}(f)$ in Proposition A.5, we get $\sigma(-J(A+B+\mathrm{H}ess\,\mathfrak{h}(f))) \subset i\mathbb{R}$. $\square$

We end this appendix with a specific nonlinear Hamiltonian for which Noether's theorem ([Arn][AbMa]) can be stated in a very explicit form.

Proposition A.8. *Assume Hypothesis A.2 with $B = 0$ and with the additional gauge invariance for $\mathfrak{h}$:*

$$\forall \alpha \in \mathbb{R}, \forall f \in \mathcal{H}, \quad \mathfrak{h}(e^{\alpha JA} f) = \mathfrak{h}(f)\,.$$

Then for any $f_0 \in D(A) \cap \mathcal{H}$, the solution f to (A.1) satisfies

$$\begin{array}{l} f \in \mathcal{C}^1(\mathbb{R};\mathcal{H}) \cap \mathcal{C}^0(\mathbb{R}; D(A)) \\ \forall t \in \mathbb{R}, \quad H(f(t)) = H(f_0) \quad , \quad (f(t)\,|\,Af(t))_{\mathbb{C}} = (f_0\,|\,Af_0)_{\mathbb{C}} \\ \mathfrak{h}(f(t)) = \mathfrak{h}(f_0) \quad \textit{and} \quad \|f(t)\| = \|f_0\|. \end{array}$$

Proof: The new gauge invariance implies that for any $f, \varphi \in \mathcal{H}$ and $\alpha \in \mathbb{R}$:

$$\begin{aligned} \mathfrak{h}(f) + (\nabla\mathfrak{h}(f)\,|\,\varphi) + O(\|\varphi\|^2) &= \mathfrak{h}(f+\varphi) = \mathfrak{h}(e^{\alpha JA}(f+\varphi)) \\ &= \mathfrak{h}(e^{\alpha JA} f) + \left(\nabla\mathfrak{h}(e^{\alpha JA} f)\,|\,e^{\alpha JA}\varphi\right) + O(\|\varphi\|^2) \\ &= \mathfrak{h}(f) + \left(e^{-\alpha JA}\nabla\mathfrak{h}(e^{\alpha JA} f)\,|\,\varphi\right) + O(\|\varphi\|^2)\,. \end{aligned}$$

Hence we get

$$\forall f \in \mathcal{H}, \forall \alpha \in \mathbb{R} \quad , \nabla\mathfrak{h}(e^{\alpha JA} f) = e^{\alpha JA}\nabla\mathfrak{h}(f)\,.$$

Thus the solution to (A.1) with $f_0 \in \mathcal{H}$, $f(t) = \Phi(t) f_0$, also satisfies

$$\forall \alpha \in \mathbb{R}, \forall t \in \mathbb{R}, \quad e^{\alpha JA} f(t) = \Phi(t)(e^{\alpha JA} f_0)\,.$$

The regularity of the flow with respect to initial data allows to say that for any $t \in \mathbb{R}$, $e^{\alpha JA} f(t)$ is differentiable with respect to α when $f_0 \in D(A)$. This yields

$$(f_0 \in D(A)) \Rightarrow \left(f(.) = \Phi(.) f_0 \in \mathcal{C}^0(\mathbb{R}; D(A))\right)\,.$$

Proposition A.4 gives

$$\forall t \in \mathbb{R}, \quad H(f(t)) = H(f_0)$$

when $f_0 \in D(A)$. It is enough to check that the quantity $(f(t) \,|\, Af(t))$ does not vary. By differentiating the new gauge invariance with respect to α we get now for any $g \in D(A) \cap \mathcal{H}$:

$$0 = \frac{d}{d\alpha}\mathfrak{h}(e^{\alpha JA} g)\big|_{\alpha=0} = (\nabla \mathfrak{h}(g) \,|\, JAg) \ .$$

For $f(t) = \Phi(t) f_0$ with $f_0 \in D(A) \cap \mathcal{H}$ we compute:

$$\begin{aligned}
\partial_t \left(f(t) \,|\, Af(t) \right) &= 2\,\mathbb{R}\mathrm{e}\,(\partial_t f \,|\, Af(t)) \\
&= 2\,\mathbb{R}\mathrm{e}\,(-JAf(t) \,|\, Af(t)) + 2\,\mathbb{R}\mathrm{e}\,(-J\nabla \mathfrak{h}(f(t)) \,|\, Af(t)) \\
&= 0 + 2\,(\nabla \mathfrak{h}(f(t)) \,|\, JAf(t)) = 0 \,.
\end{aligned}$$

Finally, the fact that $\|f(t)\| = \|f_0\|$ is a direct consequence of the equality $\mathfrak{h}(e^{\alpha J} f) = \mathfrak{h}(f)$.
□

Remark A.9. *For the specific Hamiltonian considered in Proposition A.8, one can think about several criteria for the formal stability and the nonlinear stability. This would require additional discussions and again specific assumptions according to [HMRW]. We do not consider such criteria in our analysis.*

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